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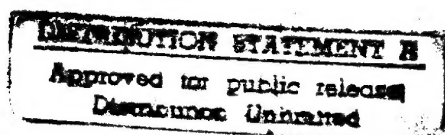
MAFELAP 1996

Conference on

THE MATHEMATICS OF FINITE ELEMENTS AND APPLICATIONS

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SUMMARIES OF PAPERS

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MAFELAP 1996

This booklet contains the abstracts of all papers presented at MAFELAP 1996. The abstracts are listed in alphabetical order of first author of each paper:

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A MATHEMATICAL MODEL OF GRAIN VENTILATION

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The theme of this communication is to give mathematical model, it's numerical solving algorithm for grain cooling process with ambient air in bins. Using basic laws of physics we obtain the following system of four partial differential equations which contain grain and air temperature ($\Theta(x, t)$ and $T(x, t)$), grain moisture $W(x, t)$ and air humidity $d(x, t)$:

$$\frac{\partial W}{\partial t} = K(W_p - W), \quad t > 0, \quad x > 0 \quad (1)$$

$$\frac{\partial d}{\partial t} + a_1 \frac{\partial d}{\partial x} = \frac{K}{a_2}(W - W_p), \quad t > 0, \quad x > 0 \quad (2)$$

$$\frac{\partial \Theta}{\partial t} = c_1(T - \Theta) + c_2(W_p - W), \quad t > 0, \quad x > 0 \quad (3)$$

$$\frac{\partial T}{\partial t} + a_1 \frac{\partial T}{\partial x} = c_0(\Theta - T), \quad t > 0, \quad x > 0 \quad (4)$$

where x, t are the variables of layer thickness and cooling time.

Initial conditions for the system (1)–(4) are given constant, boundary conditions indicate average temperature and humidity of atmosphere in August–September during the last ten years in Latvia. They are:

$$T_{x=0} = 15 + 3.5 \sin\left(\frac{\pi}{12}(\tau_d - 9.6)\right), \quad d_{x=0} = 82.5 + 15 \sin\left(\frac{\pi}{12}(\tau_d + 2.4)\right)$$

where τ_d – light hour ($0 \leq \tau_d \leq 24$).

The system (1)–(4) is solved by difference scheme using weights σ_k . The stability of schema is given.

The simulation is used for three types of grain moisture, it's corresponding tolerable max. temperatures and with two light conditions $\tau_d=2$ pm and 4 am. The results show that effective removal of moisture by means of temperature gradient is little dependent on grain moisture at the beginning and light conditions τ_d and take place in the first 30–40 minutes. It is 2–3 times shorter than the one which is considered at present. The influence of different atmospheric air filtration speed on the grain temperature and moisture conveyance in the cooling process is analyzed.

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A MAXIMUM PRINCIPLE FOR TIME DEPENDENT NEUTRON TRANSPORT THAT ENSURES WITH DISCONTINUOUS TRIAL FUNCTIONS LOCAL NEUTRON CONSERVATION IN THE MOST GENERAL WAY WITH RESPECT TO SPACE, TIME AND DIRECTION

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A typical trial function for this maximum principle of the first-order time dependent Boltzmann equation for neutron transport is discontinuous with respect to position, directions and time. Finite elements can be used to specify the positional and temporal dependencies of the trial function. For its directional dependence practical representations use either spherical harmonics or discrete ordinates. The variational solution provided by the principle ensures that neutron conservation holds locally for every space-time element with respect to every positional and temporal shape function, and for every moment used in the directional representation of the trial function. Simple illustrations of the principle are given.

The potential advantages of a conserving finite element method for neutron transport are discussed for current nuclear safety investigations. In these studies the nuclear induced fluid motion of a system with a free surface is treated by the Navier-Stokes equation.

TOWARDS AN ADAPTIVE PARALLEL *HP* FINITE ELEMENT ALGORITHM FOR ELLIPTIC PDES

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The theory needed for an adaptive parallel finite element algorithm will be discussed. Such an algorithm requires a number of components:

- a suitable a posteriori error estimator and refinement strategy to adaptively decide whether to refine the element geometry (h -refinement) or the polynomial degree of the element (p -refinement).
- a data structure supporting arbitrary non-uniform h -refinements and non-uniform p -refinement of the polynomial degree in each element and in each component of the solution.
- a solution algorithm for the linear system of equations which simultaneously tackles the problem of ill-conditioning of the system and harnesses the power of the parallel architecture.

The paper will present recent theoretical progress on these problems and outline how the theory is translated into a practical algorithm. Numerical examples will be included illustrating the performance of the algorithm for the adaptive, parallel solution of elliptic systems.

OPTIMIZATION OF MAGNETIC DEVICES USING FINITE ELEMENT ANALYSIS

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In the design of magnetic devices the use of Finite Element Analysis is becoming increasingly widespread, to allow a deeper understanding and control of the magnetic field features which influence the overall performance. However, when the results of an analysis put into evidence a disappointing performance, the usual approach is that the designer should devise possible changes to some device parameters, perform a new analysis, evaluate the new performance, and iterate the procedure by hand until satisfactory results are achieved.

A possible way to improve this approach is that of letting the designer define a set of parameters that could be modified, prescribing for each of them upper and lower limits and allow them to assume continuous or discrete values. An Objective function computable on the basis of the results of a Finite Element Analysis of the

device should then be devised, defining in mathematical terms the RperformanceS that has to be improved, minimizing or maximazing the objective function in the allowable subset of the parameter space. So defined, the procedure lends itself, if the Finite Element code is provided with adequate flexibility and robustness, to an automatic loop that, from a given starting point, automatically performs changes to the set of parameters and new analyses until a satisfactory result is reached. This approach, though simple to define in principle, poses a series of algorithmic and computational challenges, since objective function values associated to each set of parameters can be computed only after each Finite Element Analysis and do not allow an easy and general definition of reliable local values of derivatives. A number (up to some hunfreds) of analyses are usually required to find even the closest local minimum with a deterministic strategy, that should be selected among those allowing to reach the minimum with the smallest number of function evaluations. The situation is of course much more demanding for the definition of global minima, that have to be searched for by means of stochastic approaches.

In the paper an overview of the most frequently used deterministic and stochastic approaches to face this class of problems is provided, their features are briefly reviewed, some techniques to accelerate convergence are described and the most significant lines of development are outlined.

ON HIGHER ORDER MIXED FEM FOR NAVIER-STOKES FLOWS

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ADDRESS NOT SUPPLIED

We consider following nonlinear elliptic equations with Neuman condition at the boundary.

$$a_0(x) - 2\mu \operatorname{div} \epsilon(u) + Dp = f(x)$$

$$\operatorname{div}(u) = 0.$$

$$u = 0.$$

Here u is velocity vector, p represents pressure, $\epsilon(u)$ is the symmetric part of the velocity gradient. f is the given body force and μ is viscosity. a_0 is a piecewise constant. We follow the method of [2] and utilise Babuska-Brezzi condition for K-ellipticity.

Our aim is to obtain stability and consistency of the solution. This method enhances the stability of solution which is consistent as exact solution. This in turn satisfies the variational equation.

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APPLICATION OF THE DUAL RECIPROCITY METHOD TO THE SOLUTION OF HELMHOLTZ EQUATION

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Recently the *Dual Reciprocity Method* (DRM) has been proposed as a way of extending the boundary integral equation method to a large class of second order nonlinear and inhomogeneous boundary value problems of the type

$$\nabla^2 u = f(x, y, t, u, \nabla u, \partial u / \partial t) \quad (1)$$

(see [2]). The method is based on approximating the right hand side *source* term by a finite sum of special distance functions v_i , where $v_i = \nabla^2 \psi_i$, in order to obtain a boundary only integral equation. These distance functions belong to the larger class of *radial basis functions* (rbf); see [3].

In this paper we propose to apply the DRM to the solution of Helmholtz equation written in the form of (1) with $f = -k^2 u$. We expect this technique to offer some advantages over the classical boundary integral equations for the Helmholtz equation (see [1, 4] and references therein). Matrices will be frequency independent which should result in efficiency gain in problems of practical interest where the solution is required for a range of values of the wavenumber. Furthermore, the spurious non-uniqueness problem associated with the classical boundary integral equations for the exterior Helmholtz problem may be overcome.

Numerical results will be presented for the classical boundary integral equations and those from DRM.

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A REVIEW OF FAST ALGORITHMS FOR BOUNDARY INTEGRAL EQUATIONS.

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Discretisation of boundary integral equations in general lead to fully populated complex valued and non-hermitian systems of linear equations. The cost of setting up the boundary element system is approximately $c_1 n^2$ with c_1 moderate to large whilst its solution by multi-grid or methods from the Krylov subspace class such as CGN, BCG, CGS or GMRES, perhaps after appropriate preconditioning, requires approximately $c_2 n^2$ operations, with c_2 small to moderate.

Over the last decade a number of faster algorithms such as multipole expansion [5], panel clustering [4], wavelet expansion [1, 6], multilevel [2], impedance matrix localisation [3], capable of solving the boundary integral equations in $\mathcal{O}(n \ln^d n)$, with d having some small value, have been proposed.

In this paper we review these fast methods and aim to present some experimental results on their relative efficiencies. The design of appropriate preconditioners will also be discussed.

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THE SYMMETRIC GALERKIN BOUNDARY ELEMENT METHOD IN 3D ELASTICITY

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A boundary value problem in three-dimensional linear elasticity is solved via a system of boundary integral equations. A Galerkin approximation of both strongly singular and hypersingular boundary integral equation is considered, leading to a symmetric system of linear equations.

The evaluation of *Cauchy* principal values (v. p.) and finite parts (f. p.) of double integrals is one of the most difficult parts within the implementation of such boundary element methods.

The numerical cubature of these integrals is discussed in the case of domains which have piecewise smooth surfaces with a Riemann metric structure. The integration method presented leads to explicitly given regular integrand functions which can be integrated by standard Gaussian product quadrature. Problems of a wide range of integral kernels on curved surfaces can be treated by this integration method. We give estimates of the quadrature errors of the singular four-dimensional integrals.

Because the effort for the analytical evaluation of the integrands of the element stiffness matrices increases with the complexity of the kernel functions and with the polynomial degree of the shape functions, the computer algebra system "Maple V" ¹ was used for this task. A "Maple V" program greatly simplifies the implementation of this new integration method especially for matrix-valued kernel functions.

We compare the theoretical results with numerical computations.

IMPROVED FINITE-VOLUME-TYPE METHODS FOR CONVECTION-DIFFUSION PROBLEMS

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A well-known effect in the application of usual finite volume schemes to convection dominated diffusion problems is that interior layers resulting, for example, from discontinuous data on the inflow boundary, are perceptibly smeared in directions perpendicular to the characteristics (crosswind direction).

To overcome this disadvantage, an upwind finite volume method with adaptive choice of control volumes is proposed. The key idea is to build such control volumes

¹MAPLE is a registered trademark of Waterloo Maple Software

the shape of which depends on the the convective field. An analysis of the artificial diffusion terms shows that, for a fixed distribution of nodes, the proposed scheme yields a diminished crosswind diffusion in comparison with other finite volume schemes.

Numerical examples of upwind methods with both Voronoi volumes and adapted volumes are given.

REFINEMENT OF FINITE ELEMENT MESHES NEAR CORNERS AND EDGES

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The solution of elliptic boundary value problems has singular behaviour of r^α -type near concave corners and edges. This results in lower accuracy of standard discretization techniques in those critical regions, especially in a lower convergence order. Because of the practical importance of such problems there have been developed adapted numerical methods to increase the approximation to the optimal order. Here, we shall deal with finite element methods involving local a-priori mesh refinement.

Because of the importance of the exponent α , possibilities of its computation are discussed. Then an isotropic mesh refinement strategy is described for the treatment of two- and three-dimensional problems. However, near anisotropic structures as edges it seems to be natural to use anisotropic meshes. A-priori error estimates will be reviewed for both types of meshes.

A STABILIZED GALERKIN METHOD ON SHISHKIN-TYPE MESHES FOR CONVECTION- REACTION- DIFFUSION PROBLEMS

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The numerical solution of the convection-reaction-diffusion problem is considered in a bounded domain in two and three dimensions. A stabilized finite element method of Galerkin/ Least-squares type accomodates diffusion-dominated as well as convection- and /or reaction-dominated situations. The resolution of boundary layers occuring in the singularly perturbed case is accomplished using anisotropic mesh refinement in boundary layer regions.

In this paper, the standard analysis of the stabilized Galerkin method on isotropic meshes is extended to more general meshes with boundary layer refinement. The critical point of such estimates is an assumption on the Sobolev norms of the solution which is hard to prove in the general case. In particular, we consider meshes of so-called Shishkin-type. Simplicial Lagrangian elements of arbitrary order are used.

We present some numerical examples and address the question of appropriate iterative solvers for the arising discrete problems.

The results are partly published in [1] .

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DOMAIN DECOMPOSITION METHODS FOR CONVECTION-DOMINATED PROBLEMS

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In the first part, we present some results on domain decomposition methods for convection dominated convection-diffusion problems. Two different parallelizable Schwarz type methods are considered. The first method is of overlapping type. In the singularly perturbed limit, we prove linear convergence of the continuous domain decomposition method provided that the given flow field is simple. The second method is the fictitious overlapping technique (by P.L. Lions) or the equivalent augmented Lagrangian method (by P. Le Tallec). We obtained optimal efficiency in both cases using stable discretization methods together with inexact solution of the subproblems. In the second part of the paper, we apply the proposed methods to the incompressible Navier-Stokes problem together with stable discretization methods of upwind type. We obtained fairly good results for the overlapping method in simple examples as driven cavity flow in 2D and 3D and Reynolds numbers up to 10^4 . The results with the nonoverlapping method are less promising so far. Other nonoverlapping variants are still under consideration.

NEW PROBLEMS AND TRENDS IN THE FINITE ELEMENT METHOD

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Engineering decisions today are more and more based on the computational analysis of mathematical problems which by assumption describe well the engineering reality. The finite element method gives an approximate solution or the particular data of interest extracted from this solution.

The finite element approach has to be adaptive with reliable a-posteriori error estimation of the data of interest. Assuming that this is achieved, it still does not guarantee that a reliable engineering decision can be made. This is because the mathematical model can be unreliable either because of its formulation or because of the unreliability of the input data. Hence the unavoidable uncertainties should be a part of the mathematical problem.

The main problems today seem to be:

- a) The proper formulation of mathematical problems incorporating the uncertainties in the available information.
- b) Design of the method for solving mathematical problems, methods which are robust and can treat well the problems, e.g. with unsmooth solutions (due to interfaces), or highly oscillatory, as in the Helmholtz problem.
- c) A-posteriori error estimation of the data of interest and adaptive procedures with quantitative, theoretical, and computational characterization of their quality.

The lecture will present a survey of some problems and trends touching the above problems; for example:

- a) Mathematical problems of reliability of formulation of cyclic plasticity in conjunction with experiments.
- b) Formulation of the problems with uncertain data.
- c) The new partition of unity finite element method (PUFEM).
- d) Some aspects of the h - p version of the finite element method.
- e) Mathematical and numerical aspects of the reliability of the a-posteriori error estimation, the adaptive procedure, and pollution error.

MONOTONE ITERATION METHODS FOR SOLVING DIFFERENTIAL AND INTEGRAL EQUATIONS

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The discretization of linear or nonlinear partial differential equations using the finite difference or finite element method leads to very large but sparse systems of linear or nonlinear equations. Those can be solved either by classical iteration methods like SOR- or SOR-Newton-method or by multigrid method [3]. Especially in the nonlinear case it is favourable to compute the iterates monotonically, because then the existence of sub- and supersolutions guarantees the convergence of the sequences without any extensive convergence theory [4]. Moreover, one gets automatically an inclusion of the computational error.

Using the multigrid method we can prove that it converges monotonically whenever the smoother does [2]. Because most of the common smoothers can be computed monotonically, too, we have a lot of possibilities to construct monotone multigrid schemes for systems with an L-structure. Together with the introduction of transferred testvectors this result can be applied also to the frequency filtering method [1], [5].

Numerical results show that the monotone including algorithm particularly in the non-linear case will be quite fast, especially with an adaptive determination of a correction parameter matrix, which weights the defect correction. Because of the robustness of the ILU-iteration the monotone frequency filtering method can be used profitably to solve anisotropic problems with a small parameter ε [1].

The idea of monotone enclosure can also be transferred to integral equations if the computational domain can be coarsened in a natural way. In this case the matrix of the linear system will not be sparse. Nevertheless, the monotone multigrid scheme is an efficient solver for a sufficiently large number of gridpoints.

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PREDICTING DEFECTS IN FIBER OPTIC CABLES

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This paper presents a modelling study into predicting defects that occur within optical fibers during the fabrication process of submarine cables. This form of transmission media is required for sending high quality data between continents. Manufacturing these cables involves heating a copper clad steel core that is surrounded by a plastic coating. A number of fiber optic strands are then pressed into this plastic coating and then passed through an extruder where extra heated plastic material is moulded around the fibers to form the inner part of the cable. This assembly is then passed through two cooling troughs and then coiled. During this fabrication process inbuilt stresses arise in each of the fibers due to the thermal gradients set up throughout the cable. If the difference between the principle stresses, ie. Birefringence, at any point is relatively large then the performance of the fibers in transmitting clear signals will be limited. Microbending is also a result of poor fiber processing where small curvatures occur within the fiber which result in transmission losses. Optimising a cables performance with regards both birefringence and Microbending losses involves obtaining a greater understanding of the mechanisms that are present in the fabrication process. This paper shows how computational mechanics is being used to help gain a greater understanding of this process.

PARALLEL ADAPTIVE MULTI-GRID: THE SOFTWARE TOOLBOX UG

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We discuss the development and practical application of a flexible algorithmic concept and a corresponding software toolbox for multi-grid methods on unstructured and locally refined grids. This toolbox allows the application of adaptive methods and modern optimal multi-grid solvers with robust smoothers and algebraic coarse-grid correction to a wide variety of problems from continuum mechanics. Special emphasis is put on the parallelization of the toolbox. This implies the development of automatic dynamic load balancing algorithms. The efficiency and reliability of the concept for practical computations is demonstrated for several applications from structural and fluid mechanics.

A PARALLEL SOLUTION TECHNIQUE FOR STRUCTURAL PROBLEMS IN STATICS AND DYNAMICS

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The substructure technique is an appropriated tool for the finite-elemente-analysis of very complex problems in structural mechanics, even on computers with small high speed memory (RAM) and slow peripheral storage media (harddisk). Due to the natural parallelism of the reducing processes and the computation of the internal displacements by backward substitution on each substructure, the substructure technique is well suited for parallel computing ([1]). A decisive influence on the efficiency of the implementation is given by the solving algorithm of the main system of equations. The common used direct and iterative solvers have some disadvantages. A good load balancing for parallel processing is difficult to obtain and the iterative solvers often require good preconditioning.

This paper presents an explicite solving algorithm for structural problems in dynamics, which especially can be used for effective solving of engineering problems in statics and its implementation on parallel computers. Considering static problems, the equation

$$K \cdot u = F$$

is a special case of the dynamic problems

$$M \cdot \ddot{u}(t) + C \cdot \dot{u}(t) + K \cdot u(t) = F$$

under the additional condition

$$\ddot{u}(t) \equiv \dot{u}(t) \equiv 0.$$

The solution of this differential equation can be obtained without generating the stiffness matrix K by using this explicite solving algorithm. While using a diagonal mass matrix not only computing time can be saved but considerably memory space. Furthermore, a good load balancing is obtained easier caused by the independence of the bandwidth of the stiffness matrix. Hence, it is independent of the numbering of the unknowns of the equation.

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A FEM APPROACH FOR THE ANALYSIS OF OPTIMAL CONTROL OF DISTRIBUTED PARAMETER SYSTEMS USING A MAXIMUM PRINCIPLE

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Distributed control, as well as boundary control, are effective means for suppressing excessive structural vibrations. By introducing a quadratic index of performance in terms of displacement and velocity, as well as the control force, it is possible to determine the optimal control. This optimal control is expressed in terms of an adjoint variable by utilizing a maximum principle. With the optimal control applied, the determination of the corresponding displacement and velocity is reduced to solving a set of differential equations involving the state variable, as well as the adjoint variable, subject to boundary conditions, initial conditions and terminal conditions. This set of equations may, in general, not be separable and easily solved. Furthermore, the computational effort to determine the analytical solution may also be excessive. Presented herein are finite element numerical algorithms which easily solve the set of equations for both optimal distributed and optimal boundary control problems in a space-time domain for the case of the Euler-Bernoulli beam. Using these finite element recurrence schemes, numerical results for various beam configurations are presented which compare the behavior of the controlled and uncontrolled systems and are also compared with the analytical results for some test cases.

BRIDGES BETWEEN THE FINITE ELEMENT METHOD AND COMPUTER AIDED GEOMETRY

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Energy methods (ie variationnal ones in FEM), are popular in CAGD, mainly for surface editing . It is thus natural to try to import in this domain some of the paradigms of the Finite Element Method. In our current research we have used the concept of hierarchy in h and p elements and general 2D paving, as well as "isoparametricity" to build an effective new kind of surface, based on classic Bézier patches.

Higher order continuity is obtained by using a duality method based on Lagrange multipliers, leading in a natural way to mortar type meshes. Hierarchy is used to get an efficient sparse matrix solver.

The present construction is a new kind of surface which is defined by an under-

lying “logical unstructured mesh” + a corresponding isoparametric parameterization + local Bézier functions.

We illustrate our approach on some complex meshes, consisting of thousands of quadrilateral elements and some hole filling procedures in homage to Gregory.

Now if the FEM contributes to CAGD the reverse is also true. In some cases (boundary surfaces for adaptive 3D meshes), the tangents must be properly approximated and a geometric regularity kept, the best way to do that is to use CAGD methods. Higher order curved elements meshes can be generated thus giving first order regular isoparametric transformations. Moreover by using the isoparametric extension of local Bézier functions and for instance a fourth order operator one can build C1 numerical approximation for plates or shell that uses the surface geometric regularity concepts, sometime easier to implement than the parametric regularity ones. And this can be done in an H - P hierarchical setup. Examples from CAD and FEM will illustrate our method.

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ADAPTIVE REMESHING WITH FINITE ELEMENT METHODS FOR TIME-DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

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A common approach to finding numerical solutions to time-dependent partial differential equations (PDEs) is to use the method of lines (MOL). This technique involves reducing an initial boundary value problem (IBVP) to a system of ordinary differential equations (ODEs) in time through the use of a

discretization in space, using the finite element method (FEM) for example. The system of ODEs, which takes the form of an initial value problem (IVP), can then be solved using standard adaptive software. In this paper we consider the effect of using adaptivity in space, as well as time, by allowing the finite element discretization to alter as the solution evolves. In particular, we focus on the common situation where

the adaptivity in space occurs at discrete times (using h-refinement for example) and therefore leads to discontinuities in the corresponding ODE system.

By applying this approach to the solution of the 2-d compressible Navier-Stokes equations for unsteady external flows about an aerofoil, we will demonstrate that if such discontinuities are not treated carefully they can cause the efficiency of the ODE solver to be drastically reduced through the use of unnecessarily small time steps and low order integration formulae. We will also demonstrate that these inefficiencies can arise for simpler one-dimensional test problems, which we are able to analyse. This analysis, which considers the effects of different strategies for the interpolation of solution data between meshes (after remeshing has occurred) allows us to explain the demonstrated behaviour – and to suggest the most reliable strategies for interpolation between meshes.

SOLUTION OF LARGE 3D PLASTICITY PROBLEMS

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Plasticity problems are mostly solved by incremental finite element algorithms which divide the load history into load increments and define the displacement, strain and stress increments from the requirements of force balance under given plasticity conditions. Using the finite element approximation, these algorithms lead to the solution of system of nonlinear equations within each load increment.

For large 3D plasticity problems, the main computational effort is involved in the solution of the large scale nonlinear systems. It can be performed by various techniques, but in our paper, we shall concentrate only on Newton and Newton-like methods with inexact solution of the auxiliary linear systems. Inexact solution here means solution by some efficient iterative method using some lower accuracy. This accuracy must be sufficient for the convergence of the Newton-like or Newton technique and must guarantee that we do not waste a lot of the computational effort in solving auxiliary linear systems.

In our paper, we shall present some recent theoretical convergence results concerning inexact Newton and Newton-like methods [2], [1] as well as some experience from performed numerical experiments, see [3].

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ON LOCAL COUPLING AND DEFECT CORRECTION TECHNIQUES IN THE NUMERICAL TREATMENT OF SINGULARITIES

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The efficient numerical solution of elliptic PDEs involving local singularities usually requires local modifications of standard finite element discretization schemes. We discuss several strategies of coupling such local modifications with standard global methods which lead to schemes of optimal order of convergence. In particular, an iterative approach similar to Hackbusch's local defect correction method is discussed. The coupling approach may also lead to more efficient solution schemes for the resulting algebraic equations compared, for instance, to global adaptive mesh refinement strategies. In particular, we discuss the different treatment of polluting and non-polluting singularities like, e.g., corner singularities and singularities induced by concentrated forces.

ON THE ROTHE'S - MIXED FINITE ELEMENT METHOD FOR THE QUASISTATIONARY VON KÁRMÁN'S EQUATIONS

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We consider the system of integro-differential equations describing large deflections of a thin viscoelastic plate. The system contains a second-kind Volterra integral equation with respect to the Airy stress function and a pseudoparabolic equation for the deflection. They are connected by nonlinear terms :

$$H_{ijkl}(0)\partial_{ijkl}\Phi(t) + \int_0^t \partial_t H_{ijkl}(t-s)\partial_{ijkl}\Phi(s) ds = -h[\partial_t w, w], \quad (1)$$

$$\frac{h^3}{12}(A_{ijkl}^{(1)}\partial_t\partial_{ijkl}w + A_{ijkl}^{(0)}\partial_{ijkl}w) - [\Phi, w] = f(t), \quad (2)$$

$$\Phi(t, \xi) = \frac{\partial\Phi}{\partial\mathbf{n}}(t, \xi) = w(0, x) = w(t, \xi) = \frac{\partial w}{\partial\mathbf{n}}(t, \xi) = 0, \quad (3)$$

$$[v, w] = \partial_{11}v\partial_{22}w + \partial_{22}v\partial_{11}w - 2\partial_{12}v\partial_{12}w. \quad (4)$$

$$t \in [0, T], \quad x = (x_1, x_2) \in \Omega \subset R^2, \quad \xi \in \partial\Omega;$$

The initial-boundary value problem (1)–(4) can be expressed in a weak form: to find $\{\Phi, w\} : [0, T] \rightarrow V \times V$, $V = H_0^2(\Omega)$; such that:

$$H(0)\Phi(t) + \int_0^t \partial_t H(t-s)\Phi(s) ds = -h[\partial_t w(t), w(t)], \quad (5)$$

$$A_1\partial_t w(t) + A_0w(t) - [\Phi, w] = f(t), \quad (6)$$

$$w(0) = 0 \quad (7)$$

with the operators $H(t), A_0, A_1$ operating from V into V^* .

There exists a solution $\{\Phi, w\}$ of the problem (5), (6), (7). Applying the Rothe's method with respect to the time variable t we achieve the semidiscrete form of (5), (6), (7):

$$H_0\Phi_i + \tau \sum_{j=1}^i \partial_t H_{i+1-j}\Phi_{j-1} = -\frac{h}{2}\partial[w_i, w_i], \quad \Phi_0 = 0, \quad (8)$$

$$A_1\partial w_i + A_0w_i - [\Phi_i, w_i] = f_i, \quad w_0 = 0, \quad (9)$$

$$\partial w_i = \frac{1}{\tau}(w_i - w_{i-1}), \quad \tau = \frac{T}{n}, \quad f_i = f(i\tau), \quad i = 1, \dots, n. \quad (10)$$

The existence of a solution $\{\Phi_i, w_i\} \in V \times V$ of the system (8), (9) can be verified using the same arguments as in the case of stationary von Kármán's equations. The mixed finite element method will be used in the space discretization of (8), (9).

MODELLING MAGNETIC LEVITATION CASTING USING CFD TECHNIQUES.

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It is necessary in the casting of reactive metals such as Titanium alloys which are increasingly used in the Aerospace industry to avoid contact between the metal and the crucible. Magnetic levitation, where the liquid metal is supported by an external magnetic field is an attractive method used for this purpose. In this investigation, a configuration where a moving coil is used to melt a metal ingot and also laterally supported is modelled using CFD techniques. The coupled equations describing the magnetic field, and the induced fluid motion in the melting metal together with the Enthalpy equation characterising the change of phase are solved. A general curvilinear mesh is used to discretise the equations, and since the shape of the liquid free surface is computed during the calculation from the balance of hydrostatic, magnetic and surface tension forces on it, the mesh is adjusted at each time step to follow the free surface position. Axisymmetric results only are available at present, although 3D simulations are planned for the future.

A NUMERICAL INVESTIGATION OF THE INTERACTION OF ADJACENT COOLING TOWER PLUMES

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An investigation has been conducted on the interaction of adjacent cooling tower plumes issued into an oncoming atmospheric boundary layer. The governing equations of the conservation of momentum, continuity and thermal energy are solved on a Cartesian body-fitted grid using a finite volume method.

Both wind tunnel and full scale situations are modelled. The small scale wind tunnel model utilises a low Reynolds number turbulence model together with the compressible Navier- Stokes equations where density is calculated from the equation of state. The full-scale model employs three turbulence models, namely the standard k-e, the renormalised group theory (RNG) k-e and a differential flux turbulence model. Two discretisation schemes are used to integrate the governing equations in both small and full scales. These are the hybrid scheme as well as the third order accurate

QUICK scheme. For the latter case a bounded form of the QUICK scheme is used, CCCT QUICK, for the turbulent kinetic energy and transport equations to ensure positive values for these two variables at all times.

The work studies the effect of both discretisation scheme and turbulence model on the predicted plume trajectory and spreading. The mechanisms by which adjacent plumes interact when the sources are positioned side-by-side and in tandem with respect to the oncoming crosswind are analysed. The ratio of the plume source to cross wind velocity is also varied and the subsequent interaction trends are studied.

ERROR ESTIMATION FOR THE FINITE ELEMENT SOLUTION OF THE HELMHOLTZ EQUATION

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1. Introduction. Research on error estimation for finite element discretisations has become very popular mainly for elliptic or parabolic PDE. Among the techniques studied in the literature, the error in constitutive law, initiated by P. Ladevèze *et al.* [2], has the advantage to guarantee that the estimated error is an upper bound of the exact error. It is the purpose of the present contribution to show how this estimator can be applied to acoustics for linear triangles and to study the frequency dependance especially near the eigenfrequencies.

2. Model problem. The acoustic problem is addressed by the Helmholtz equation ($\Delta p + k^2 p = 0$ where $k = \omega/c$ is the wave number) and the appropriate boundary conditions. The link between the gradient of pressure and the velocity is derived from the motion equation ($-j\rho\omega v = \nabla p$) and will be called here the constitutive law by analogy with structural mechanics. The Helmholtz equation leads to an eigenvalue problem except if ω has a prescribed value. In this case, the solution corresponds to a harmonic forced response.

3. Admissible solution. The error estimation in constitutive law is based on the solution of the admissible problem defined by the Helmholtz equation and the boundary conditions. The admissible solution does not satisfy *a priori* the constitutive law and the corresponding residual defines a measurement of the error. The full paper will give an extensive description of the developments required to construct these admissible fields.

4. Upper bound property. The errors are measured in the L^2 norm (for complex variables). It can be shown that the estimated error bounds asymptotically ($h \rightarrow 0$) from above the exact error.

5. Influence of the eigenvalues. Most acoustic analysts consider ω as a parameter and the error estimation should remain reliable in the neighbourhood of the finite element eigenfrequencies. The error estimation based on the Zienkiewicz and Zhu superconvergent patch recovery technique does not strictly fulfill this last condition [1]. It is the purpose of the present paper to show that the estimation in constitutive law still satisfies the upper bound property near the eigenfrequencies.

6. Concluding remarks. The full paper will show that the numerical tests on

both academic and industrial examples confirm the good performances of the error estimation based on the constitutive law.

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REFINED MIXED FINITE ELEMENT METHODS FOR THE STOKES PROBLEM

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We show that the solution to the Stokes system with Dirichlet boundary conditions in a polygon or a polyhedron belongs to suitable weighted Sobolev spaces. This regularity leads to optimal rates of convergence for some mixed finite element methods refined judiciously near the singular points. Similar results were obtained in the references hereafter.

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ON THE AXISYMMETRIC STOKES FLOW WITH CORNER SINGULARITIES

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We study the Stokes flow in tubes with abrupt changes of the diameter. Our first concern is the asymptotic behaviour of the solution near the corners. Then we show some consequences on the numerical method used.

We consider the rotational symmetry of the problem. This allows us to restrict to 2-dimensional problem using the cylindrical coordinates r, z . The stream function ψ satisfies then the equation

$$(1) \quad \frac{1}{r} \left(\frac{\partial^4 \psi}{\partial z^4} + 2 \frac{\partial^4 \psi}{\partial z^2 \partial r^2} + \frac{\partial^4 \psi}{\partial r^4} \right) - \frac{1}{r^2} \left(\frac{\partial^3 \psi}{\partial z^2 \partial r} + \frac{\partial^3 \psi}{\partial r^3} \right) + \frac{1}{r^3} \frac{\partial^2 \psi}{\partial r^2} - \frac{3}{r^4} \frac{\partial \psi}{\partial r} = 0.$$

This equation is different from that for the stream function in the disk geometry, where the asymptotic behaviour of the solution near the corners is known (cf. eg. [2]). In our paper we transform the equation into the polar coordinates ρ, θ and study the equation

$$(2) \quad S_0(\psi) \equiv \frac{\partial^4 \psi}{\partial \rho^4} + \frac{2}{\rho^2} \frac{\partial^4 \psi}{\partial \rho^2 \partial \theta^2} + \frac{1}{\rho^4} \frac{\partial^4 \psi}{\partial \theta^4} = 0.$$

Using the technique of Fourier transform and some of the results of [2], we obtain the asymptotic behaviour of the stream function ψ near the corner. Eg. for the internal angle of $\frac{3}{2}\pi$ we have

$$\psi(\rho, \theta) = \rho^{1.72513} \varphi(\theta) + \dots,$$

which means that the velocity components v_1, v_2 behave near the corner like

$$v_i(\rho, \theta) = \rho^{0.72513} \varphi_i(\theta) + \dots$$

These asymptotics are different from those obtained for the planar Stokes flow.

Our results enable us to adapt the finite element mesh near the corners. We present also some numerical results based on our approach suggested in [1].

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NUMERICAL ASPECTS OF NON-LINEAR FLOW EQUATIONS IN THE INVERSE PROBLEM FRAMEWORK

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The solution of non-linear transient flow equations (e.g unsaturated or multiphase) requires iterative methods. The number of iterations demanded for convergence often depends on time step size (it increases when step size increases). On the other hand, use of small time steps increases the total number of solution times and, therefore, the global cost. In other words, minimization of the cost requires a compromise between time step size and iteration number demanded per each solution. Since the numerical characteristics of each problem may vary extensively, a general and efficient set of rules for adopting optimal time step sizes is not possible in practical cases.

Surprisingly, the above limitations are greatly reduced when an additional difficulty is added to the problem: solving the simulation in the frame of the inverse problem. The reason is that inversion forces one to solve the physical problem several times under similar conditions (inverse looks for optimal physical parameters which reproduce real responses of the system modeled). Thus, an efficient algorithm, in this case, can be defined taking advantage of the following observations: I- General trends of the physical (direct) problem solution do not vary dramatically from one to the next inverse iteration. Therefore, initialization is based on the fact that the absolute change of the state variable between two solution times remain very similar from one inverse iteration to the next (it verifies in most of the cases). II- The coarsest time step discretization which allows convergence is similar for two consecutive inverse iterations. Therefore, storing the time discretization at the current inverse iteration is usefull in order to anticipate time step requirements in the next one, avoiding many computations. III- Accuracy of the simulation solution may be relaxed during several inverse iterations because those solutions are only part of intermediate results. This allows us to use relaxed criteria when inverse problem state is far from convergence and to restrict them when it is near.

Results obtained after testing various algorithm alternatives report attractive savings in the direct computational cost. A remarkable conclusion of the testing exercise is that the resulting algorithm becomes very versatile and flexible.

ON ADAPTIVE FEM FOR THE RELAXED DOUBLE-WELL MINIMIZATION PROBLEM

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The minimization of non-convex energy functionals is motivated in the mathematical theory of material science to describe phase changes (we refer, e.g., to works by Ball and James). A scalar model example is the so-called double-well functional defined by $W(F) := |F - F_1|^2 \cdot |F - F_2|^2$ where the wells $F_1 \neq F_2$ are prescribed and $F = \nabla u$ is the deformation gradient. The model problem under consideration is Problem (P): *find a minimizer $u \in \mathcal{A}$ of*

$$I(u) := \int_{\Omega} W(\nabla u) dx + \alpha \cdot \|u - f\|_2 + \int_{\Omega} g \cdot u dx.$$

Here, f and g are given functions in $L^2(\Omega)$, Ω a given Lipschitz domain, $\alpha \geq 0$, and \mathcal{A} is a closed subspace of $W^{1,4}(\Omega)$ to describe possible Dirichlet boundary conditions. It is well-known that Problem (P) may have infinite solutions or no (classical) solution. It is shown in a recent work by Carstensen and Plechac that the relaxed problem (RP), defined by replacing W by its convex envelope W^{**} , saves enough information to obtain the global displacement field, described the oscillations observed in minimizing sequences in the Problem (P) and recovers the global stress field.

The talk gives an overview about theoretical and numerical results obtained so far for (RP) and discusses further refinements for adaptive mesh-refinements.

AN INTEGRATED APPROACH FOR THE DESIGN, ANALYSIS AND MANUFACTURABILITY ASSESSMENT OF SHEET METAL PARTS

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At MAFELAP 1990 we introduced a new feature-based computer aided design method for designing functional parts like sheet metal car inner panels. With this method, a designer can directly and smoothly assemble and represent a complex, multi-featured surface using simpler component surfaces and information about feature shape. At MAFELAP 1996 we will focus on analysis and manufacturing issues related to downstream processing of inner panel surfaces designed by our feature-based approach. In particular, we will discuss (1) how structural properties of a panel design are evaluated with the aid of finite element analysis tools (for example, automatic mesh generation), (2) how finite element formability analysis is used to evaluate manufacturability issues associated with a proposed design, and (3) how the feature-based design paradigm can be used to efficiently generate NC tool centers for milling die face surfaces used to produce the part. In this presentation we do not describe anything new in CAD/CAE/CAM technology. Rather, we will illustrate the value of integrating these technologies to permit a tighter coupling between the activities of part design, part analysis and part manufacturability assessment. Although our application emphasis is rather narrow (stamped sheet metal products), the design, analysis and manufacturability issues that prevail in that area occur to one degree or another in many other industrial applications.

PANEL METHODS IN SPORTS AERODYNAMICS - RACING CARS

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The aerodynamics of a racing car is one of the most important factors which determine its performance. First a streamlined body is necessary to minimise the aerodynamic drag. Second, a racing car engine can manifest its high power only if the wheels exercise a sufficiently firm grip on the road. For this reason, components such as the front wing and the rear spoiler must provide very strong aerodynamic downforce. Third, sufficient airflow must be directed into the radiators to maximum heat transfer. Until very recently the aerodynamics design of racing cars has largely been based on experimental studies in the wind-tunnel.

In the last couple of years, computational aerodynamics has gained popularity

among many Formula-One teams. Because of the nature of the industry, the designers are required to analyse a large number of models of highly complex geometry in a matter of months, sometimes weeks. The panel method (boundary element method) prevails over full Navier-Stokes solvers in both mesh generation and problem solving. And, indeed, most Formula-One teams do not have the computational resources to use a full Navier-Stokes solver.

It has to be realised that the panel method provides a potential flow solution and thus cannot predict phenomena such as skin friction and flow separation. Therefore an integrated computational-experimental approach has been adopted by many teams. First the computation reduces the amount of experimental work required while the experiments can provide information, such as flow separation, that the panel method cannot.

The integrated strategy that we have been using at Exeter in conjunction with Formula-One teams is as follows. First, when a new set of regulations has been published, the preliminary design of the front wing and the rear spoiler can be carried out using a two-dimensional complex variable panel method package. The designer can test a vast number of proposed configurations. The most promising designs are selected and a three-dimensional source/doublet panel method with vortex wake relaxation can then be used to analyse the entire car assembly. A small number of designs are then selected for wind-tunnel and then road tests. Based on the feedback of the experimentalists and the drivers, the designer can easily modify the computational model and do the three-dimensional calculation again. The iterative process can go back and forth a few times between the experimentalists and the numerical analysts. Such a strategy largely reduces the amount of expensive wind-tunnel time required. In this presentation, some numerical aspects of the methods used will be discussed.

NUMERICAL MODELLING OF THE MULTIPHYSICS SHAPE CASTING PROCESS

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For a computer model to be successful in the metal shape casting, the complete casting process needs to be addressed, the principle physical phenomena of the process being:- filling of the hot liquid metal into a mould cavity; solidification and evolution of latent heat in the liquid metal; convection currents in the liquid metal generated by thermal gradients; deformation of the cast and residual stress development in the solidified metal; and the formation of macroscopic porosity. These events combine the analysis of fluid dynamics, solid mechanics and a change of phase. None of these events can be treated in isolation as they inexorably interact with each other, usually in a complex way. Coupled this with complex geometries, common in aerospace and automobile applications, even with simple shapes, the inclusion of running system, location of risers and chills will inexorably make it complex. In this presentation, the numerical modelling computing code PHYSICA is used to model and to address the multiphysics phenomena that is present in the metals casting process.

A NEW TECHNIQUE FOR IMPROVING MESH IRREGULARITY

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This paper presents a new technique that is to be used before smoothing a mesh.

Within any initial mesh there may be some non-ideal interior nodes which have more or less than six boundary lines. The non-ideal node will produce irregularities which need to be reduced in order to produce a hexagon. Recent study shows that in some cases, some meshes will not stabilise at the neutral threshold (T) when it equals to 2. That is the edge swapping activities oscillate indefinitely between edges connecting the 7,5-pair or 7,6-pair or 5,6-pair of points, and the irregularities cannot be reduced further.

Our proposal is based on the mesh relaxation and point placement. We present some cases where the mesh irregularity can be minimised even at the neutral threshold $T = 2$. The technique is implemented in single convex domains. The result shows that in some cases, our proposal can minimise mesh irregularity.

RATE OF CONVERGENCE ESTIMATES FOR THE SPECTRAL APPROXIMATION OF A GENERALIZED EIGENVALUE PROBLEM

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The aim of this work is to derive rate of convergence estimates for the spectral approximation of a mathematical model, which describes the vibrations of a

solid-fluid type structure. First, we summarize the main theoretical results and the discretization of this variational eigenvalue problem. More precisely, we deal with a quadratic eigenvalue problem involving incompressible Stokes equations. In its numerical approximation we use Lagrange finite elements with degree 2 (velocity) and degree 1 (pressure) polynomials on triangles. Then, we state some well known abstract theorems on spectral approximation and apply them to our specific problem, which allow us to obtain the desired spectral convergence. Under classical regularity assumptions, we are able to establish estimates for the rate of convergence of the approximated eigenvalues and the gap between generalized eigenspaces. The nume-

rical results obtained confirm the theory, as they show in particular that the known theoretical bound for the maximum number of non-real eigenvalues admitted by such a system is optimal and that we have the well known result of super-convergence for the behaviour of approximated eigenvalues.

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OSCILLATIONS OF A SQUARE PLATE CENTRALLY HIT BY A PULSE OF PROTONS

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The work presented is part of a feasibility study for a neutron spallation source planned by the European Union. Neutrons emerge as a result of a nuclear reaction when a pulsed beam of high energy protons is directed on a target. Obviously, the target is a crucial component in the design of the neutron source. Not only is there a large amount of heat deposited by the beam of protons but also heating of the target material occurs during an extremely short time interval. As a result thermal shock waves are expected, and a calculation was performed to clarify the situation whether the stress waves are critical with respect to fracturing the target or not.

The calculations were performed with a *finite-element* code called Femfam. It is an in-house development using for dynamic analyses the method of modal decomposition of stiffness and mass matrices. The geometry of the target was chosen to be a square plate made from tantalum with the dimensions $2 \times 100 \times 100 \text{ mm}^3$. The stress waves caused by one single proton pulse are represented by means of video tape and television set showing 6 sequences of moving pictures. The 6 sequences show the oscillations which occur with quite different frequencies, and they show the time dependent stress distributions of the various components of the 3D stress tensor. A scale of colors is used to indicate the amount of stressing throughout the target.

More specific results of the calculation are the frequencies which range in between 18.5 kHz and 1.35 MHz, the displacement amplitudes ranging in between $0.45\ \mu m$ (across plate thickness) and $6.0\ \mu m$ (in-plane), and the amplitudes of the stress waves ranging from -59 to 51 N/mm^2 .

COMPUTATIONAL ISSUES IN THE MODELLING OF MATERIALS

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The Manufacture of materials products involves the control of a range of interacting physical phenomena. The material to be used is synthesised and then manipulated into some component form. The structure and properties of the final component are influenced by both the interaction of the continuum scale phenomena with those at an atomistic level. Moreover, during the processing phase there are some properties that cannot be measured (typically at the liquid-solid phase change). However, it would appear there is the potential to derive properties and other features from atomistic scale simulations that are of key importance at the continuum scale. Some of the issues that need resolving in this context focus upon computational techniques and software tools to facilitate :

- 1) The multiphysics modelling at the continuum scale.
- 2) Coupling between atomistic through microstructural to continuum scale.
- 3) Exploitation of parallel computing.

This paper will discuss some of the attempts to address each of these issues particularly in the context of materials processing for manufacture.

OPTIMAL DESIGN OF ELECTRICAL MACHINES BASED ON 3D FINITE ELEMENT METHOD

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The Finite Element Method (FEM) in the recent years has been found as a very attractive in the design, especially an optimal design, and an analysis of electrical machinery and electromagnetic devices. In the paper a methodology for numerical modelling of 3D magnetic field calculation and a performance analysis of different types of electrical machines will be presented. A suitable mathematical model and an original algorithm for the nonlinear and iterative calculation by using finite element method (FEM) in 3D domain of the electrical machine will be given. Three dimensional model of the analysed electrical machines enables to take into consideration the different configuration along the three axes, including the domain outside of the machine, too. The programme package FEM-3D will be used to perform automatically mesh generation of the finite elements in the 3D domain, calculation of the magnetic field distribution, as well as electromagnetical and electromechanical characteristics in electrical machines of different types.

In this paper will be presented an algorithm for the optimisation of the design of electrical machines, on the basis of the three dimensional - 3D calculation of the magnetic field. It is started from the Maxwell's equations for the distribution of magnetic field. The distribution of the magnetic field is expressed by the nonlinear differential equation known as Poisson's or Laplace's equation. An algorithm and an original programme package FEM-3D for application of the finite element method for calculation of 3D magnetic field in electrical machines, by using a personal computer will be developed. The programme package FEM-3D, is used to perform: automatically mesh generation of the finite elements in the 3D domain, calculation of the magnetic field distribution, as well as electromagnetical and electromechanical characteristics of electrical machines. The programme package FEM-3D has been successfully applied to different electrical machines. Examples of three applications are given later, as follows.

Switched Reluctance Motor - A nonlinear iterative calculation of the magnetic field in the switched reluctance motor 8/6 poles will be performed quasistatically for different excitation currents in the stator windings and different rotor angular positions along one pole pitch. The magnetic field distribution for the rated excitation current and at the maximum permeance of the rotor will be presented on the three levels in the full paper. Having the distribution of the magnetic vector potential in the whole investigated domain from the three dimensional magnetic field calculation of the switched reluctance motor, the main flux is determined, as well as leakage fluxes in the stator windings, i.e.: the leakage flux in the active parts of the windings and in the winding overhangs, too. The optimisation of the design of the switched reluctance motor will be carried out by changing the saliency of the rotor.

Permanent Magnet Motor - The programme package FEM-3D will be also

used for an analysis and optimisation of the permanent magnet synchronous motor. The magnetic field distribution in different cross sections at rated load will be presented in the full paper. The knowledge of electromagnetic torque characteristics is very important matter for analysis and performance of electrical motors. In this paper the energy concept for numerical calculation of electromagnetic torque is applied and for the permanent magnet motor it will be calculated by the change of the magnetic system coenergy at virtual angular displacement of rotor, for constant value of current in the excitation windings. The optimisation of the permanent magnet motor will be based on the change of the torque with the shape and the value of the permanent magnet excitation.

Solid Salient Pole Synchronous Motor - Complex calculations and both an analysis and optimisation of the solid salient pole synchronous motor will be performed by the programme package FEM-3D, too. The modelling and simulation of the motor is particularly adjusted to take into consideration the movement of the rotor. The calculations of the magnetic flux distribution will be carried out for different armature currents at rated excitation current, changing the rotor position in reference to the selected initial position. Having the distribution of the magnetic vector potential in the whole investigated domain obtained from the three dimensional magnetic field calculation of the motor, the magnetic flux density is calculated. The improvement of the distribution of the air-gap magnetic flux density in the solid salient pole synchronous motor will be carried out by changing the pole shape.

FINITE DIFFERENCE METHODS APPLICABLE TO THE DESCRIPTION OF INJECTION MOULDS

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Injection moulding is a processing technique widely used in the polymer industry. The cooling stage represents an important part of the entire production cycle and the thermal interaction between the mould, the polymer part, the cooling water inside the mould (when present) and the environment affects the rate at which heat is dissipated from the polymer. Overall, such a complex interaction will control both the productivity (cooling time) and the moulding quality. This may result from unbalanced cooling which leads to great variations in the thermal profiles along the periphery and subsequent distortions in the final shape. Usually, these two basic requirements are of difficult compromise.

In order to assess the various operating parameters, a model was implemented to describe the transient behaviour of the moulding coupled with the mould. The heat diffusion equation was discretized over the computational domain using a finite difference technique. This is suitable for a great variety of moulding geometries often found in the industry. Appropriate boundary conditions for the polymer/mould interface (where high thermal gradients occur) were derived based on an energy balance. In addition, Neumann boundary conditions for the internal cooling channels and the environment were coupled with appropriate convective heat transfer coefficients.

The effect of the various operating conditions (water temperature and flow rate), geometric parameters (channel layout, part thickness) and material properties on both the cooling time and the temperature distribution along the part periphery was investigated for a variety of shapes: flat, U and T shaped parts. Amongst the various conclusions, it is observed that for thicker parts, complex shapes and longer cooling times the heat flux follows a more complex pattern than that assumed when 1D transient analysis is employed (Fig. 1). Taguchi techniques were applied to determine quantitative relationships between the various parameters and the mould performance. Generally, higher productivity rates are coupled with larger temperature differences along the part periphery and such an effect is more severe for the more complex shapes.

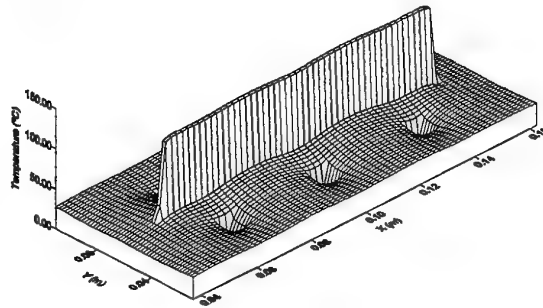


Fig. 1

2D FEM ANALYSIS IN 3D DESIGN OPTIMISATION OF A HOMOPOLAR PMG

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The analysed synchronous homopolar permanent generator (PMG) consists of a stator with a permanent magnet and two polar pieces carrying the stator coils and a rotor ferromagnetic armature with skewed crenels. With a 2D based technique we solve the 3D magnetic field problem of the PMG operated under no - load condition, by determining the resulting magnetic flux through the stator coils as well as the induced electromotive force (EMF), corresponding to different skewings of the rotor crenels. Practically, we have analysed a cross-section of the synchronous homopolar PMG. The solving of magnetostatic field problem, formulated in the terms of the magnetic vector potential, was performed for 20 relatively different positions of the two armatures which move with a constant interval of 1.5 deg (the rotor crenel pitch is 60 deg). Supposing the rotor crenels are unskewed, the magnetic flux through a stator coil, for a relative k positions of the armatures, is given by the relation of magnetic fluxes (the difference between the MVP along the slots axis where the coils sides lie, multiplied by the number of turns and the ideal machine length, too. In order to take into account the rotor crenels skewing, supposing that the magnetic flux density has no component along the axial axis, it is necessary to solve the problem of a finite number of the two armatures relative positions, n , and then to calculate the average of the solutions along the axial direction (n is the ratio between the skewing angle and the displacement constant interval). The induced EMF is calculated by taking into account, one after the other, the average fluxes differences corresponding to successive positions according to the displacement constant interval divided with the time interval (the displacement constant interval divided by pulsation). In conclusion, the paper presents a 2D FEM based technique for a 3D design optimisation of the resulting magnetic flux through the stator coils and the induced EMF of a synchronous homopolar PMG. Thus, the sinusoidal form of the terminal induced voltage curve of the machine was obtained for a skewing angle of the rotor crenel of 22.5 deg.

PARALLEL IMPLEMENTATION AND ANALYSIS OF A FINITE ELEMENT METHOD FOR SURFACE WATER FLOW

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Sophisticated finite element models have been developed for surface water flow. Gray, Kolar, Luettich, and Westerink have developed a semi-implicit Galerkin method based on combining the momentum equation with the generalized wave continuity equation. Numerical experimentation indicates that this model is robust, accurate, suppresses spurious oscillations, and allows for grid flexibility.

The model was developed for implementation on scalar and vector platforms. Using domain decomposition techniques, we have parallelized this program for distributed memory parallel computers. We will discuss details of this implementation and its performance on several test problems.

We have also analyzed this numerical model for stability and accuracy. A priori error estimates have been derived for a continuous time Galerkin formulation. These estimates are currently being extended to include various time-stepping schemes and boundary conditions. The results of this analysis will also be discussed.

We are currently investigating new algorithms based on different time-stepping approaches and approximating spaces. Second-order time-stepping approaches such as those developed by Rannacher, et al, combined with mixed approximating spaces for velocity and elevation are being considered. These schemes will be compared to the method of Gray et al for accuracy and parallel efficiency.

SOLUTION OF VISCOELASTIC SCATTERING PROBLEMS BY MEANS OF *HP*-ADAPTIVE BE/FE METHODS

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The presentation focuses on steady state scattering problems, describing interaction of an acoustical fluid with elastic and viscoelastic bodies. The presentation will focus on practical issues connected with the use of *hp* - Adaptive Finite Element discretizations, including:

- compatibility of Boundary Element (BE), and Finite Element (FE) approximations,
- a - posteriori error estimation for coupled BE/FE approximations,
- mesh optimization strategies. Several numerical results will illustrate the presented methodology.

FINITE AND BOUNDARY ELEMENT METHODS IN ACOUSTICS - A COMPARISON

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The presentation focuses on the numerical solution of the Helmholtz equation in exterior domains. Two numerical strategies are discussed: Boundary Element (BE) and Infinite Element (IE) Methods. The first strategy is based on replacing the Helmholtz equation, together with the Sommerfel radiation condition, with an equivalent Burton - Miller boundary integral equation. The equation is then formulated in a weak form, allowing for a convenient Galerkin approximation by boundary elements. The second approach is based on a direct weak formulation for the original Helmholtz equation, followed by an approximation using infinite elements. The presented discussion will focus on both mathematical and practical, numerical issues, including convergence analysis, stability (with respect to the wave number), cost comparison, and numerical verification.

A NUMERICAL METHOD FOR THE COMPUTATION OF THE DISPERSION OF A CLOUD OF PARTICLES BY A TUBULENT GAS FLOW FIELD

K. Domelovo and L. Sainsaulieu

ADDRESS NOT SUPPLIED

The paper is concerned with the construction of a numerical method for the computation of the dispersion of a cloud of liquid droplets by a turbulent gas flow field. The cloud of droplets is modeled by a semi-fluid system intermediate between a fluid model and a kinetic description of the dispersed phase. The semi-fluid model is deduced from the kinetic model by integration with respect to the velocity variables and allows to describe clouds of particles such that the velocity distribution of any family of particles with a given radius and a given temperature, found at a given location of the physical space is a gaussian function. A numerical scheme, consistent with the semi-fluid model and inspired from Perthame's or Deshpande's kinetic schemes is proposed. The interactions with the gas phase are taken into account thanks to a Particle in Cell method. Numerical experiments enlight the features of the method.

The whole paper is available as a compressed Postscript file by internet procedure FTP anonymous on host `barbes.polytechnique.fr` (129.104.4.100) in the directory `pub/RI/1996` under the name

`domelevo_sainsaulieu_343.mai.ps.gz`

or by Xmosaic or any other www client via the CMAP www server

A 2D FINITE ELEMENT METHOD FOR MAGNETIC ANALYSIS USING A VECTOR HYSTERESIS MODEL

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A numerical model based on a single valued material characteristic doesn't show the phase difference between the magnetic flux density \mathbf{B} and the magnetic field strength \mathbf{H} in the case of a rotating magnetic flux excitation. This rotating magnetic flux excitation in electrical machines results from the complexity of the magnetic circuit and of the magnetic motoric force distributions.

In this paper we present the inclusion of the vector Preisach model, as described in [1], in the magnetic field calculations in a 2D-domain D . This domain D represents one tooth region of the stator of an asynchronous machine. The magnetic behaviour of the material can be described in terms of the macroscopic fields, taking into account the hysteresis phenomena.

Writing $\bar{\mathbf{H}} = -\text{grad}\varphi$ for the magnetic field $\bar{\mathbf{H}} = H_x\bar{\mathbf{i}}_x + H_y\bar{\mathbf{i}}_y$, the scalar potential φ is found to obey the following PDE:

$$\frac{\partial}{\partial x} \left(\mu_{xx} \frac{\partial \varphi}{\partial x} + \mu_{xy} \frac{\partial \varphi}{\partial y} \right) + \frac{\partial}{\partial y} \left(\mu_{xy} \frac{\partial \varphi}{\partial x} + \mu_{yy} \frac{\partial \varphi}{\partial y} \right) = 0 \quad (1)$$

where the coefficient functions $\mu_{xx}, \dots, \mu_{yy}$, arise from the relations

$$B_x = \mu_{xx}H_x + \mu_{xy}H_y \text{ and } B_y = \mu_{xy}H_x + \mu_{yy}H_y \quad (2)$$

between the magnetic induction $\bar{\mathbf{B}} = B_x\bar{\mathbf{i}}_x + B_y\bar{\mathbf{i}}_y$ and the magnetic field $\bar{\mathbf{H}}$. These relations result from the vector Preisach model. The functions $\mu_{xx}, \dots, \mu_{yy}$ depend on $\bar{\mathbf{H}}$ and $\bar{\mathbf{H}}_{past}$.

The boundary ∂D is divided into six parts $\partial D_1, \partial D_2, \dots, \partial D_6$. On ∂D_i , $i=1,2,3$ the normal component of $\bar{\mathbf{B}}$ vanishes while on the remaining parts

$$\int_{\partial D_i} \bar{\mathbf{B}} \cdot \bar{\mathbf{n}} dl = \phi_i(t) \text{ (enforced) and } \varphi = C_i(t) \text{ (unknown) }, i = 4, 5, 6. \quad (3)$$

The demagnetized state of the material leads to a zero scalar potential φ at $t = 0$ throughout D .

This complex boundary value problem is solved numerically by a suitable FEM.

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SOME ASPECTS OF THE NUMERICAL SOLUTION OF 3D STEFAN PROBLEM IN HETEROGENOUS MEDIA

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Simulation in geodynamics often requires phase transitions or recrystallization processes being introduced to the models. Also, with still more powerful computers being available, it became possible to construct and solve real models in 3D.

In the article, the Stefan problem in 3D with dissipative heat term will be investigated. The algorithm will be presented and different solution methods of arising nonlinear system considered.

Presented method is a part of a system, created for the purpose of investigation of geodynamical systems, e.g. models concerning long-time safety of the radioactive waste repositories.

ADAPTIVE GRID REFINEMENT WITH A HIGH RESOLUTION SCHEME FOR AQUIFER REMEDIATION IN THREE DIMENSIONS

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Reservoir simulation and (environmental) aquifer remediation involve solving a coupled system of essentially hyperbolic conservation laws (for fluid transport) and an elliptic equation for the pressure. The coupling between the equations is via the fluid velocity, which is defined by Darcys law to be proportional to the pressure gradient.

Accuracy of numerical results from any simulator can be improved by performing global mesh refinement, which typically has to be repeated several times to obtain a "converged" result. A single global 3D refinement can increase the computation time and requirements by at least a factor of eight excluding timestep restrictions. For many problems, regions of interest with large flow gradients occupy only a small percentage of the flow domain, and therefore the ability to perform local mesh refinement in regions of interest is highly desirable; benefits of increased accuracy and reduced computational cost are achievable when combining grid adaptivity with higher-order schemes [3, 4].

This paper presents a description of the adaptive scheme discretisation based on adaptive implementation in UTCHEM a general purpose chemical flooding simulator [2]. An application to a three dimensional remediation problem is presented [1]. There are two stages to the problem: The first stage involves a spill, where the pollutant (a dense non-aqueous phase liquid DNAPL) is injected into an aquifer and allowed to distribute under gravity and according to globally imposed flow gradient across the domain. The pollutant occupies a relatively small region of the domain

and this process provides an excellent opportunity for testing local mesh refinement. The second stage involves the remediation process. Surfactant is injected into the aquifer through several strategically placed wells in order to recover the pollutant. Benefits of local mesh refinement are illustrated in this very important problem.

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COMPUTATION OF THE LIMIT LOAD OF AN ELASTOPLASTIC STRUCTURE

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Under the plane stresses hypothesis, we consider an elastoplastic structure occupying a bounded regular domain $\Omega \subset \mathbf{R}^2$, governed by the Hencky law and submitted to a density of forces λf acting on Ω and a density of forces λF acting on a part Γ_F of the boundary Γ of Ω ; $\lambda \in \mathbf{R}$ is the loading parameter. The displacement field u satisfies $u = u_0$ on the part Γ_U of Γ . The limit load $\bar{\lambda}$ is the upper bound of the set of λ for which the Hencky stress problem admits a solution, or equivalently, the upper bound of the set of λ for which the energy related to the Hencky problem is bounded from below. We prove in [2, 1] that $\bar{\lambda}$ is given by the new characterization :

$$1/\bar{\lambda} = \inf_{\eta \in V_\infty} \|j_K(\sigma^e - \eta)\|_{L^\infty(\Omega)} \quad (1)$$

where $V_\infty = V \cap L^\infty(\Omega; \mathbf{R}_s^4)$, $V = \{\eta \in L^2(\Omega; \mathbf{R}_s^4) : \text{div} \eta = 0 \text{ in } \Omega, \eta \nu = 0 \text{ on } \Gamma_F\}$, K is the elastic convex set, j_K the gauge function of the convex K and σ^e is the stress field solution of the elastic problem. When using (1) to compute the limit load $\bar{\lambda}$, the L^∞ norm is an important source of numerical difficulties. In order to overcome this difficulty, we suggest the regularization of the functional appearing in (1), by introducing the following real sequence :

$$1/\bar{\lambda}_q = \inf_{\eta \in V_q} \|j_K(\sigma^e - \eta)\|_{L^q(\Omega)} \quad (2)$$

where q is a real satisfying $q \geq 2$ and $V_q = V \cap L^q(\Omega; \mathbf{R}_s^4)$. Then, we prove in [2, 1] that

$$\bar{\lambda} = \lim_{q \rightarrow +\infty} \bar{\lambda}_q.$$

In order to compute the limit load $\bar{\lambda}$ as a limit, when $q \rightarrow +\infty$, of $\bar{\lambda}_q$, we use a non conforming finite element method based on Morley finite element. Let $M_h^0(\Gamma_F)$ be the Morley finite element space, we introduce the discrete Airy operator \mathcal{A}_h and the discrete space $V_h = \mathcal{A}_h(M_h^0(\Gamma_F))$. Then, we introduce for a fixed q :

$$1/\bar{\lambda}_{q,h} = \inf_{\eta_h \in V_h} \|j_K(\sigma_h^e - \eta_h)\|_{L^q(\Omega)} \quad (3)$$

where σ_h^e is the solution of the discrete elastic problem; and we prove in [2] that $\bar{\lambda}_q = \lim_{h \rightarrow 0} \bar{\lambda}_{q,h}$. Therefore, the limit load $\bar{\lambda}$, given by (1), satisfies $\bar{\lambda} = \lim_{q \rightarrow +\infty} \lim_{h \rightarrow 0} \bar{\lambda}_{q,h}$. This method is tested on a beam submitted to a traction effort with a Von-Mises elastic convex. The error is less than 3%.

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ITERATIVE METHODS FOR DISCRETE MAXWELL EQUATIONS

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The computational cost of the finite element solution of the 3D time-harmonic Maxwell equations is dominated by that of solving the resulting large sparse linear system of equations. Particularly in high-frequency scattering applications, these systems become so large that direct solvers are no longer an option and iterative methods must be used. In this talk we focus on 3D cavity problems as well as scattering problems discretized using the first-kind Nédélec edge elements. We give an overview of preconditioned Krylov subspace methods – currently the most powerful class of iterative algorithms for large and sparse linear systems – which can be applied to the resulting non-Hermitian system and demonstrate their effectiveness on several test problems.

DISCRETE-TIME ORTHOGONAL SPLINE COLLOCATION METHODS FOR SCHRÖDINGER EQUATIONS IN TWO SPACE VARIABLES

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Consider the initial-boundary value problem (IBVP) for the Schrödinger equation in the unit square Ω

$$\frac{\partial \psi}{\partial t} - i\Delta \psi + i\sigma(x, y, t)\psi = f(x, y, t), \quad (x, y, t) \in \Omega \times (0, T],$$

$$\psi(x, y, t) = 0, \quad (x, y, t) \in \partial\Omega \times (0, T],$$

$$\psi(x, y, 0) = g(x, y), \quad (x, y) \in \Omega,$$

where $\partial\Omega$ denotes the boundary of Ω , $i^2 = -1$, Δ is the Laplacian, σ is a given real nonnegative function, and f and g are given complex-valued functions. Problems of this type arise in many applications in quantum mechanics, underwater acoustics, plasma physics and seismology.

In this paper, we briefly overview existing techniques for solving the IBVP, and introduce two new discrete-time orthogonal spline collocation methods. These are Crank-Nicolson and alternating direction implicit (ADI) schemes employing C^1 piecewise polynomials of degree ≥ 3 . For each scheme, we outline the derivation of stability and the proof of optimal order *a priori* estimates in the L^2 - and H^1 -norms. We also describe the parallel implementation of the ADI method and discuss the extension of the methods to other Schrödinger-type problems.

THE THEORY AND APPLICATIONS OF NUMERICAL SCHEMES FOR NONLINEAR CONVECTION-DIFFUSION PROBLEMS AND COMPRESSIBLE NAVIER-STOKES EQUATIONS

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Numerical simulation of viscous compressible high-speed flow belongs to one of the most difficult areas of Computational Fluid Dynamics, because all significant obstacles are concentrated here: convection dominating over diffusion, shock waves, boundary layers, their interaction and, on the other hand, the lack of theoretical analysis of the continuous problem. Our goal is to develop a robust theoretically based numerical method for the solution of viscous compressible flow applied on unstructured meshes, with the emphasis to the investigation of aerodynamical properties of blade machines.

The viscous terms in the system of governing equations consisting of the continuity equation, Navier-Stokes equations and energy equation are considered as a perturbation of the inviscid Euler equations. Therefore, the method is based on a general class of flux vector splitting cell centred finite volume schemes. The viscous terms are discretized by the finite element method over a triangular grid. Several combined inviscid - viscous finite volume - finite element approaches using suitable mutually consistent finite volume - finite element meshes were developed. Namely, the original triangulation is used for the conforming finite element approximation, while the finite volume method is applied on the dual mesh. Quite another finite volume - finite element approach is proposed for triangular finite volumes. In this case an adjoint finite element triangular grid is constructed to the original finite volume triangulation. Barycentric finite volumes are associated with nonconforming finite element approximation of viscous terms. In order to increase the accuracy of the scheme, adaptive flux approximation as well as adaptive mesh refinement are applied during the numerical procedure.

Substantial attention was paid to the theoretical analysis of the developed combined finite volume - finite element schemes applied to a simplified scalar nonlinear

convection - diffusion conservation law equation. Both for fully explicit and semiimplicit scheme the convergence of approximate solutions to the exact weak solution of the continuous problem was proved. The main tools in the convergence proof are the discrete maximum principle, apriori estimates and compactness arguments based on the use of the Fourier transform with respect to time. The order of accuracy was also examined. The comparison of numerical results with experimental data shows the applicability and robustness of the method.

SINGULARLY PERTURBED FINITE ELEMENTS

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Considering singularly perturbed elliptic partial differential equations of convection-diffusion type

$$-\varepsilon \Delta u + \operatorname{div}(\vec{b} \cdot u) = f \quad (1)$$

adapted finite elements may be defined by using trial and/or test functions satisfying piecewise (with respect to the finite element triangulation) an approximated equation ($\tilde{b} \approx \pm b$)

$$-\varepsilon \Delta u + \operatorname{div}(\tilde{b} \cdot u) = 0. \quad (2)$$

In the bivariate case a mixed formulation analysis of the Galerkin-Petrov discretization error of such elements is given. The influence of different methods of conforming and nonconforming fitting of the elements is discussed.

The results are applicable to some known exponential fitted finite element approximations of (1) on rectangular and triangular meshes and make possible to generalize these discretization methods.

IMPROVEMENT OF EFFICIENT AND ROBUST 3D ELEMENTS FOR THE ANALYSIS OF SOLIDS AND SHELL STRUCTURES

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Several eight node trilinear 3D solid elements based on the enhanced assumed strain (EAS) method are presented for linear elasticity and small strain plasticity. A systematic development of these brick elements for linear elasticity is briefly described, see also [2]. The proposed elements can not only be used in modelling "real" 3D problems including incompressibility and bending but also for the analysis of thin structures like shells and plates with only very few modifications.

The main focus is on element efficiency by avoiding the time-consuming static condensation of the internal strain parameters involved in the assumed strain method. This static condensation process is the main drawback of the conventional EAS-formulation [4], especially in nonlinear problems with a Newton-Raphson equation solver. The second focus is robustness: the 3D element should be able to fulfill the patch-test exactly and no hourglassing and locking should occur even in highly distorted meshes. An important advantage of the proposed element formulation is the possibility to use symbolic integration instead of the conventional eight point numerical integration. This makes it computationally as efficient as the new elements proposed by Korelc and Wriggers [3]. A comparison with the well-known B-bar elements [1] shows similarities in the linear regime whereas for nonlinear material behaviour as plasticity major differences are found to the EAS-formulation. On some numerical examples, including the simulation of thin shell structures with only one layer of elements in thickness direction, the advantages and limits of this family of enhanced assumed strain elements are discussed.

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CONTINUOUS MODELLING OF SEQUENTIAL METAL FORMING STEPS WITH INTEGRATED MICROSTRUCTURAL SIMULATIONS

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The development of a high-performance metal workpiece requires the optimisation of the whole process. That means the definition of workpiece-properties for every single process-step, from moulding and solidification to metal forming with subsequent heat treatment. Optimising these properties with large-scale experimental test series is time- and cost intensive and leads to long product cycles in industrial production.

The aim of the research-program SFB370 at the RWTH-Aachen, therefore, is a simulation program, i.e. a continuous model of the material and the whole process, which is able to substitute optimisation experiments.

Due to the historical development of most simulation-packages, which derive mainly from applied mechanics, implemented material laws are mostly restricted to an isotropic and homogeneous workpiece. Specific problems of material processing have often been neglected. An understanding of microstructural changes to a specific extent is nonetheless essential for a reliable use of models in process optimisation. For the field of metal forming, the formulation of the flow stress is of utmost importance, it is influenced to a large extent by initial microstructure and its ongoing evolution.

Hot working processes with multi-step forming operations require the simulation of microstructure changes during forming and during interstand times. For this purpose a module STRUCSIM has been developed at the Institute of Metal Forming (IBF). It computes continuously the alterations of an average grain-size proceeding from empirical Hollomon-equations and its effect on flow stress has been integrated into process simulation.

For cold working processes as well as for a coupled model of moulding and forming it is necessary to consider the effects of anisotropic material properties on flow stress. First attempts have been made together with the Institute of Metal Physics (IMM) to integrate a Taylor-model related module for the formulation of texture-evolution into the FEM-simulation of metal-forming processes. Results of the research-program and of the microstructure simulation are presented in the lecture.

ADVECTION DOMINATED TRANSPORT USING ELLAM AND TH-COLLOCATION

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The aim of this paper is to combine the Eulerian-Lagrangian Localized Adjoint Method (ELLAM) with domain decomposition, using a kind of non-conventional collocation recently proposed by Herrera (TH-collocation). As it is well known, the numerical solution of advective-diffusive transport equations is specially difficult because most numerical schemes exhibit non-physical oscillations or excessive numerical dissipation, or both. However, the ELLAM approach has shown to be very effective to treat such equation. On the other hand, domain decomposition methods are a natural route to parallelizing numerical models of continuous systems. Finally, TH-collocation has some attractive features such as relaxing the continuity conditions. Example calculations are presented to illustrate the methodology.

STUDY OF INTERPOLATION METHODS AND ITS USE IN THE ELEMENT-FREE GALERKIN METHOD. IMPROVEMENTS AND APPLICATIONS.

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The diffuse elements method, developed by Nayroles et al is a new way of discretizing the continuous media. In this method, only a mesh of nodes and a boundary description is needed to develop the Galerkin equations. The approximating function are polynomials fitted to the nodal values of each local domain by a weighted least squares approximation. Belytschko et al developed an alternative implementation using moving least square interpolants as were defined by Lancaster and Salkauskas. Liu et al has recently proposed a different kind of "griddles" multiple scale methods based on reproducing kernel and wavelet analysis. Oñate et al focused on the application of the diffuse interpolation to fluid flow problems via a standard point collocation technique. All these methods can be considered as Finite Point Methods.

The main idea of the diffuse approximation is to replace the FEM interpolation by a local weighted least squares fitting. This provides a valid approximation in a small surrounding of a point x , based on n^e nodes close to it, instead of the on-element FEM interpolation.

This allows to use a variable number of nodes in the interpolation. It is possible to disconnect the number n^e of nodes from the number m of approximation parameters because the least squares fitting replaces the standard FEM interpolation. The approximate function becomes smooth by replacing the discontinuous coefficients ($\omega_i^e = 1$ on the element, $\omega_i^e = 0$ elsewhere) by continuous weighting functions $\omega^x(x)$ evaluated at x_i . To preserve the local character of the approximation is necessary to chose weighting functions that vanish at a certain distance from the point x .

Around x , the function $u^x(x)$ is locally approximated by:

$$u^x(x) = \langle p(x) \rangle \{a^x\} \sum_{j=1}^m p_j(x) a_j^x$$

The coefficients a_j^x , corresponding to the point x , are obtained by minimizing the following expression:

$$J^x(a^x) = \sum_{i=1}^n \omega^x(x_i) (u_i - u^x(x_i))^2$$

where $\omega^x(x)$ is a positive weighting function, which quickly decreases when the distance $\|x - x_i\|$ increases.

This communication encloses a posteriori error indicator, in order to minimize the error, and a sensitivity analysis of various parameters involved. The posteriori error

indicator has been developed based on the studies of Ferragut et al. The basic idea of this error indicator is to try of distributing the error uniformly all over the domain. Each pair of evaluating points are compared in order to estimate the step in the value of the function. It has been considered than is necessary to add nodes and evaluation points when a pair of evaluation points has an error bigger than the average domain error. This procedure allows us to isolate the domain areas with a worst behaviour and refine only the small areas in the domain.

Very high rates of convergence and real saving of computer time were observed. Furthermore the method appears very effective using a posteriori error estimator. It is possible to eliminate the elements and even to dispense the evaluation points, what would permit to talk about a real Finite Point Method. This would provide a very easy preprocessing and very simple mesh adaptativity and refinement.

FICTITIOUS DOMAIN/DOMAIN DECOMPOSITION METHOD FOR VISCOUS FLOW CALCULATION

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The main goal of this presentation is to discuss the simulation of incompressible viscous flow modelled by Navier-Stokes equations by a method combining fictitious domain and domain decomposition methods.

This method allows the solution of problems associated to complicated geometries via the use of block structure measures. It is particularly well-suited to the simulation of flow with moving boundaries. The lecture will be illustrated by application to the simulation of 2-D and 3-D flows.

A NEW ITERATIVE METHOD FOR THIN PLATE SPLINE INTERPOLATION TO SCATTERED DATA

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We consider the problem of thin plate spline interpolation to n data points in general position, which are all different and which are not collinear, and where the number of data points is sufficiently large for work of $\mathcal{O}(n^3)$ to be unacceptably high. We develop the following iterative method, each iteration comprising $n - q + 1$ stages, where q is small enough for the $\mathcal{O}(q^3)$ work of thin plate spline interpolation to q data points to be sufficiently low.

We let the set V_1 be the full set of data points, V say, and for $i = 2, 3, \dots, n - q + 1$, we define the set, $V_i = V_{i-1} \setminus \{x_{i-1}\}$, where the data points are numbered in a systematic way which avoids clustering in any of the sets, V_i , and which ensures that, in each of these sets, the data points are not collinear.

At each stage, except the final stage, of an iteration, we correct our current approximation to the thin plate spline interpolant by a multiple of the Lagrange function of interpolation to a *small subset* of p data points in V_i , which are not collinear, and which include \underline{x}_i , at which data point the Lagrange function is unity. The multiplier is chosen to give a good approximation to the coefficient of the radial basis function whose centre is the data point, \underline{x}_i ; this coefficient then remains unchanged for the rest of the iteration. At the final stage of an iteration, however, we correct our current approximation to the thin plate spline interpolant by the interpolant to the residuals at the q data points of V_{n-q+1} . The iterative process continues until the maximum residual does not exceed a specified tolerance.

Each iteration has the effect of premultiplying the vector of residuals by an $n \times n$ matrix R , whose elements depend solely upon the positions of the data points, and thus convergence will occur whenever the spectral radius of this matrix is less than unity. For a number of sets of data points, and for a range of values of n , p , and q , we have found the method to exhibit fast rates of convergence.

DISTRIBUTED PARALLEL COMPUTATION FOR VISCOUS FLOWS

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This paper describes some recent developments in the parallel implementation of a transient finite element program. The application area is that of viscous incompressible flows, with particular reference to rheologically complex materials such as polymer, oils or foods. Both iterative and direct solvers are introduced within each time step cycle, based on a pressure-correction/Taylor-Galerkin algorithm. A parallel implementation is achieved using PVM over a homogeneous workstation cluster. Various parallelisation strategies based on domain splitting are investigated. These approaches may be efficiently utilised for problems on static or dynamic domains, and in two or three dimensions. Our preference is to use a direct Choleski solver for this pressure-correction algorithm. For two dimensional problems, this solver can be very time efficient and large storage requirement can be partially overcome by adopting a distributed version of the solver. However, for three dimensional and dynamic domain problems, this solver may become very inefficient and an iterative solver such as the Conjugate Gradient may be desirable. It is our intention to investigate some of these issues. Results on some test problems will be reported, where it is apparent that significant parallelism may be achieved through iterative approaches and via distribution of data and system matrix blocks.

SOLVING NON-LINEAR UNSYMMETRIC FINITE ELEMENT SYSTEMS

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Among the principal parallel algorithms, that can be classified as "Parallel Numerical Algorithms", the conversion of implicit to explicit forms offers substantial advantages because of our sequential computing experience of using the implicit methods mainly for speed and stability reasons. In this article a new class of hybrid schemes based on inner-outer iterative procedures in conjunction with the known (modified) Picard and Newton methods leading to improved composite iterative schemes for solving non-linear initial/boundary value problems. The Picard and Newton method can be coupled with direct linear solvers when the order of the finite element system is small, whereas when the order of the system is large certain class of iterative can be used. The inner solution method is based on the Extended to the Limit Generalized Approximate Inverse Finite Element Matrix (GAIFEM) techniques which are based on the concept of adaptable LU factorization. It should be noted that an important feature of these algorithmic procedures is the provision of both explicit direct and preconditioned iterative methods. Additional facilities are provided by the choice of "fill-in" (factorization) and "retention" (pseudoinverses) parameters that allow the best method for a given problem to be selected. The effectiveness of the Explicit Preconditioned iterative methods using these GAIFEM techniques for solving numerically non-linear initial/boundary value problems is related to the fact that the pseudoinverse of the original sparse coefficient matrix A (although is full) exhibits a similar "fuzzy" structure as A . The performance and applicability of the new proposed composite iterative schemata on non-linear Elliptic and Parabolic P.D.E's are discussed and numerical results are given.

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USING EXPLICIT PRECONDITIONED SCHEMES BASED ON SPARSE APPROXIMATE INVERSE FINITE ELEMENT MATRICES FOR SOLVING INITIAL VALUE PROBLEMS IN THREE DIMENSIONS

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An important achievement over the last decades is the appearance and use of Preconditioning methods for solving Elliptic and Parabolic Partial Differential Equations. Current research efforts are focused on the development of computational methods suitable for multiprocessor systems. The derivation of parallel numerical algorithms was the main objective for which several forms of approximate inverses of a finite element matrix, based on approximate factorization have been proposed. The main motive for the derivation of the approximate inverses lies in the fact that they can be efficiently used in conjunction with explicit preconditioned iterative schemes which are appropriate for solving large unsymmetric finite element linear systems on parallel and vector processors. A new class of hybrid time implicit-explicit approximating schemes combined with generalized Sparse Approximate Inverse Finite Element Matrix (SAIFEM) techniques and explicit preconditioning iterative methods for the numerical solution of initial/boundary value problems is presented. The SAIFEM techniques based on the concept of adaptable LU -type factorization procedures have been recently introduced for computing explicit pseudoinverses of large sparse unsymmetric finite element matrices of irregular structure, derived from the FE discretization of Elliptic and Parabolic Partial Differential Equations in three-space variables without inverting the corresponding decomposition factors. According to a “fish-bone” computational procedure, by using the so-called “Location-Principle” strategy, the elements of the pseudoinverse are computed by retaining $(l$ and u elements, i.e. the so-called “retention” parameters. Optimized forms of the pseudoinverse algorithm, by using a moving window from bottom to top, proved to be particularly effective for solving “banded” sparse FE systems of large order, i.e. $((l + u) < n/2$, or narrow “banded” sparse FE systems of very large order, i.e. $(\delta l + \delta u) \ll n/2$. The performance and applicability of the new proposed explicit preconditioned schemata on Singular - Perturbation (SP) time dependent linear problems are discussed by solving characteristic SP elliptic and parabolic PDE's in three-space variables and numerical results are given.

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CONCEPTS OF A FEM BLACK-BOX-SOLVER ON PARALLEL COMPUTERS

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The solution of nonlinear variational problems by the finite element method is the kernel problem for the numerical simulation of the physical systems. But the user does not want to deal with numerical aspects and implementation as far as possible, so that he can concentrate on the mathematical modeling. Therefore he asks for a *Black-Box-Solver* program package which is an optimal compromise of

- high flexibility
- easy handling
- reliability
- robustness
- efficiency.

In the talk we will discuss the design of the FEM Black-Box-Solver VECFEM, which allows the user to enter his variational problem in a symbolic representation. Especially we will consider the robustness and its consequences for optimal data structures on parallel computers.

The *Robustness* of the black-box-solver ensures that a good solution approximation is calculated for a large class of applications independent of the used computer

architecture or the *number of processors*. The nonlinear discretized variational problem is solved by the Newton-Raphson iteration, where the analytical representation of the Frechet derivative of the variational problem has to be evaluated to get a robust iteration. The resulting linear systems for the calculation of the Newton-Raphson corrections are solved by iterative methods of the conjugate gradient type. Here the matrix-vector multiplication with the sparse stiffness matrix is the key operation.

On a parallel computer the explicit availability of the stiffness matrix is essential for the robustness and efficiency of the linear solver. We will give a brief sketch of the optimal data structures for the most important subtasks:

- distribution of the mesh data
- element matrix calculation
- mounting of the stiffness matrix
- matrix-vector multiplication

An example will demonstrate how the VECFEM code generator builds up the analytical representation of the Frechet derivatives of the variational problem. The efficiency of the presented data structures is demonstrated by the performance on a parallel computer.

FINITE ELEMENT MODELLING OF HEAT FLOW DURING LASER METAL FORMING

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Lasers are used in various ways in metal fabrication industries. They have been used very efficiently for drilling, cutting and welding and now they are used for metal forming. The simulation of laser metal forming is a difficult and complicated task and in any case it has to be done in two stages. First, the problem of heat flow under a moving heat source has to be solved for the accurate prediction of the temperature distribution in the metal plate and then a thermal stress analysis has to be performed for the computation of stresses, strains and deformations.

It is of great importance to accurately predict the temperature distribution since most of the phenomena subsequently encountered, such as thermal stresses and strains, distortion, metallurgical changes, etc. have their origin in the uneven temperature distribution and the fast heating and cooling rates that occur during the laser forming of metal plates. The early attempts to solve the highly non-linear partial differential equations of heat flow and the accompanying boundary conditions where analytical but such solutions are not so accurate since several simplifying assumptions have to be made. This paper discusses the various aspects, and the degree of their complexity, of the mathematical modelling of the heat flow during the laser metal forming and presents a finite element solution.

The analysis assumes:

1. Quasi-stationary state.
2. The heat input is provided by a 3D uniformly distributed heat source moving on the surface of the plate.
3. The thermal conductivity of the material is a linear function of the temperature.
4. The thermal diffusivity of the material is constant.
5. The initial temperature of the plate can be different from the ambient temperature to allow for preheating.
6. The reflectivity of the plate is taken into account.
7. No melting or evaporation of the metal occurs.
8. Convection and radiation boundary conditions are taken into account through a constant average effective heat transfer coefficient, which can be different for the top and bottom surfaces of the plate.

Several plates of different materials which are formed to various shapes are modelled. The finite element solution is plotted against the results obtained from experiments and microhardness measurements. Deficiencies of the present model are discussed and improvements are suggested.

HOW TO USE STANDARD LAGRANGE FINITE ELEMENTS FOR SOLVING MAXWELL'S EQUATIONS

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Consider the scattering of a time-harmonic electromagnetic wave by a perfect conducting bounded obstacle. Assume for simplicity that the domain Ω surrounding the obstacle is filled by a homogeneous medium. The determination of the electric field amounts to finding the only solution $E \in H_{\text{loc}}(\text{curl}; \Omega)$ to the time-harmonic Maxwell's equations

$$\text{curl}(\text{curl } E) - k^2 E = 0 \text{ in } \Omega,$$

(where $k > 0$ is the wave number of the incident wave E^I) whose tangential component $E \times n$ vanishes on the boundary Γ of the conductor, and such that the scattered field $E - E^I$ satisfies the well-known Silver-Müller radiation condition at infinity.

Suppose that the boundary Γ is regular (C^2 say). Noticing that E is divergence-free, we deduce that $E \in H_{\text{loc}}^1(\Omega)^3$ is also a solution to the vector Helmholtz equation

$$-\Delta E - k^2 E = 0 \text{ in } \Omega.$$

It is easily seen that the converse is true provided that E is supposed to satisfy in addition a divergence-free boundary condition. More precisely, E is nothing but the only solution to Helmholtz equation which satisfies $E \times n = 0$ and $\text{div } E = 0$ on Γ , as well as the radiation condition at infinity. This property suggests a numerical method

for solving our scattering problem: instead of dealing with Maxwell's equations (using for instance Nédélec finite elements), we can equivalently solve Helmholtz equation by means of a standard discretization with nodal finite elements.

The case of an irregular boundary (e.g., a piecewise regular surface with edges and corners) is more complicated. Indeed, a similar equivalence result between Maxwell's and Helmholtz' problems can be obtained, but E has no more the $H_{\text{loc}}^1(\Omega)^3$ regularity: the solution of Helmholtz equation has to be searched for in $H_{\text{loc}}(\text{curl}; \Omega) \cap H_{\text{loc}}(\text{div}; \Omega)$, which does not allow us to use directly a standard discretization. Our aim is to show how to approximate this solution by solving two different problems. The first problem is exactly the same as for a regular boundary; its solution actually represents the "regular part" of E (i.e., the $H_{\text{loc}}^1(\Omega)^3$ part) which is computed by nodal finite elements. The second problem, which leads to the "singular part" of the E , requires a particular treatment of the singularities of the field near the singularities of the boundary.

THE FOURIER-FINITE ELEMENT METHOD: ERROR ESTIMATES, RANGE OF APPLICATION AND PARALLEL COMPUTATION

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The paper gives some survey of recent results on the Fourier-finite element method for solving Poisson-like and Lamé equations in three-dimensional domains. This method combines the finite element method with the approximating Fourier method and reduces the solution of an elliptic problem in an axisymmetric or prismatic 3D-domain to the solution of a coupled or even decoupled system of elliptic problems on the two-dimensional cross section. For the Fourier-finite element approximation, the rate of convergence in the Sobolev spaces $H^l(l = 0, 1)$ is proved to be of the order $O(N^{-(2-l)} + h^{2-l})$, where N denotes the degree of trigonometric polynomials and h the mesh size of the triangular mesh (use of piecewise linear elements). Near re-entrant corners generating re-entrant edges and singularities of the solution, appropriate mesh grading is analyzed and a priori error estimates are given. Moreover, a posteriori estimates of residual type involving the parameters N and h are considered.

Algorithmic aspects of this method and its parallelization are discussed. The results on the rate of convergence, including mesh grading, and on parallel solving elliptic problems in 3D are illustrated by numerical examples.

ON NODAL TRANSPORT METHODS

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One of the most important partial differential equations in the nuclear engineering field is the neutron transport equation in its discrete-ordinates approximation S_N which in x-y geometry reads:

$$L\psi_k \equiv \mu_k \frac{\partial \psi_k}{\partial x} + \nu_k \frac{\partial \psi_k}{\partial y} + \sigma_t \psi_k = \sigma_s \sum_{l=1}^M \omega_l \psi_l + Q_k \equiv S_k, k = 1, \dots, M, \quad (1)$$

where the unknown is ψ_k , the angular neutron flux corresponding to the k -th ray of the S_N approximation, M being the total number of rays considered which is given in this case by $N(N+2)/2$. The domain to be considered is of the union of rectangles type and boundary conditions must also be imposed.

Classically with nodal methods, the domain of interest is decomposed in relatively large homogeneous regions or "nodes", over which each angular flux ψ is approximated by a generalized interpolant with interpolation parameters which are cell and/or edge moments. This unique interpolant is piecewise continuous using polynomial (or exponential) shape functions. For a ray in the first quadrant, the possible left and bottom edge parameters are known from the boundary conditions or from the neighboring left and bottom cells. The unknowns are thus the right and top edge parameters, as well as the cell ones.

In this paper, we present two "new" classes of polynomial nodal methods. In essence, both classes of methods lead to *discontinuous* approximations. The first class however conserves one or two moments of the angular flux between the given cell and its upstream neighbors. The second class is fully discontinuous and only has outgoing (at top and right) edge moments as parameters, in addition to possible cell moments. Locally, Legendre moments of the residual $L\psi_h - S_h$ are taken to obtain as many equations as unknowns and we give criteria to pick up correctly these equations, which are actually derived over a cell which is shifted upstream by ϵ , in the limit of a vanishing ϵ . Because of the discontinuous character of ψ_h , boundary terms arise at the left and the bottom of the cell, connecting it to its upstream neighbors or to the boundary. For the first family, there may be several choices of equations, which is not the case for the second family. For both families, we have programmed all the methods from two to eight unknowns per cell and applied them to multiplicative and nonmultiplicative benchmark problems of the nuclear literature, and we compare them in the paper.

DOMAIN DECOMPOSITION METHODS: AN OVERVIEW

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This paper presents a general and updated description of the development of domain decomposition methods for partial differential equations. Both non-overlapping and overlapping decomposition are considered.

Formulations based on Steklov-Poincare operators are discussed. Also, several approaches based on Schwartz alternating procedure are explained. Recent contributions by the author -Trefftz-Herrera domain decompositions- are introduced in this overview. Applications of conjugate gradient method and its variants are also included. Different approaches to preconditioning are discussed.

THE LANDWEBER ITERATION FOR INVERSE SCATTERING PROBLEMS

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In ultra sound medicine, nondestructive testing, and several other applications the problem occurs to recover the shape of an obstacle by measurements of the far field patterns of scattered waves. Since such inverse scattering problems are nonlinear and ill-posed, difficulties arise in the numerical approximation of the shape.

We consider as an example the scattering of incoming time-harmonic acoustic wave by a sound-soft or a sound-hard infinite cylinder. Let the cross section of the cylinder be denoted by the bounded domain $D \subseteq \mathbb{R}^2$ with smooth boundary. Suppressing the time dependence leads to the exterior boundary value problem

$$\Delta u + k^2 u = 0 \quad \text{in } \mathbb{R}^2 \setminus \overline{D}$$

with a wave number $k > 0$ and the boundary condition $u = 0$ or $\frac{\partial u}{\partial n} = 0$ on ∂D in case of a sound-soft and a sound-hard obstacle respectively. The total field $u = u^i + u^s$ is the sum of the incident plane wave $u^i(x) = \exp(ikx \cdot d)$ with direction $d \in \{x \in \mathbb{R}^2 : |x| = 1\}$ and the scattered wave u^s which satisfies the Sommerfeld radiation condition.

The inverse problem under consideration consists in solving the operator equation $F(\partial D) = u_\infty$, if F denotes the operator mapping the boundary ∂D onto the far field pattern of u^s with fixed incident direction.

In the paper we derive the Fréchet derivative of F with respect to variations of the boundary which again can be represented by an exterior boundary value problem. This representation is used to obtain properties of the operator F' and also a representation of the adjoint operator if we assume for instance starlike domains.

A recent approach regularizing nonlinear ill-posed problems is the extension of the Landweber method to nonlinear problems as suggested by Hanke, Neubauer and Scherzer which consists in iterating

$$r_{j+1} = r_j + \mu F'[r_j]^*(g - F(r_j))$$

(with scaling parameter $\mu > 0$) and stop the iteration if the residual error is less than a prescribed value for the first time depending on the noise level. Here, the function r_j describes the radial component of the starlike domain D_j .

Applying the boundary integral equation method the representation of $(F'[.]^*)$ yields that r_{j+1} can be computed just by solving an integral equation of the second kind twice with different right hand sides. This leads to an efficient and stable algorithm solving the inverse scattering problem. Several incident waves can be considered just by adding up, where again the same integral equation is used. Thus we can incorporate these information nearly for free. The performance of the algorithm is discussed and illustrated by some numerical examples.

MULTILEVEL ADDITIVE SCHWARZ METHOD FOR THE $H \cdot P$ VERSION BOUNDARY ELEMENT METHOD

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We consider 2-level and multilevel methods for the $h - p$ version of the boundary element method. Both hypersingular and weakly singular integral equations of the first kind are considered. We prove that, for quasi-uniform meshes, the condition number $\kappa(P)$ of the 2-level additive Schwarz operator P grows not worse than $(1 + \log p)^2$, and not worse than $p(1 + \log p)^2$ for the multilevel method. Here p is the degree of the polynomials used in the Galerkin boundary element schemes. For the geometrically graded meshes where the condition number of the Galerkin matrix blows up exponentially in M , we show that for the 2-level method $\kappa(P) \sim O(\log^2 M)$, and for the multilevel method $\kappa(P) \sim O(\sqrt{M} \log^2 M)$. Here M is the number of unknowns of the system. Thus we show that additive Schwarz methods as a parallel preconditioner, which were originally designed for the finite element discretisations of differential equations, are also fast solvers for some boundary integral operators, which are non-local operators.

A MULTIGRID METHOD BASED ON CELL ORIENTATED DISCRETIZATION FOR CONVECTION-DIFFUSION PROBLEMS

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For the convection-diffusion equation in two dimensions we derive the cell orientated discretization which is based on the method of lines leading to differential-algebraic equations and their time integration by implicit methods. This approach is well-suited in convection-dominated cases. The efficiency of the method depends on the solution of the arising linear systems mainly. Motivated by the definiteness properties of these unsymmetric systems we choose a multigrid method with problem adapted transfer operators. The interpretation of the cell orientated discretization in a finite-volume or a Petrov-Galerkin context leads to different definitions of restriction and prolongation. In combination with smoothers which are exact solvers in the convection case (Gauss-Seidel, ILU) we achieve a robust multigrid iteration. Finally we present numerical results concerning the quality of the transfer operators as well as the various smoothing iterations. The independance of the convergence rate from the gridsize and the behaviour of various time integration schemes are also examined.

ADAPTIVE MULTILEVEL MIXED FINITE ELEMENT METHODS FOR THE MULTIGROUP DIFFUSION EQUATIONS IN REACTOR KINETICS

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The mathematical modelling and numerical simulation of the neutron kinetics is an important integral part of the safety analysis of nuclear reactors. For the sake of an efficient and cost-effective simulation, the multigroup neutron diffusion theory is commonly used instead of the more exact but expensive transport theory. In mathematical terms, the multigroup diffusion equations represent an eigenvalue problem for a coupled system of parabolic equations where the eigenvalue corresponds to the critical constant of the reactor. Since nuclear engineers are interested in both the neutron fluxes and the neutron currents, the use of mixed finite elements for discretization in space is considered as an appropriate approach.

In this contribution, we present a fully adaptive mixed finite element scheme featuring a combined step-size control in time and adaptivity in space. In particular, we use a mixed hybrid approach based on the lowest order Raviart-Thomas-Nédélec elements with respect to an adaptively generated hierarchy of hexahedral triangulations of the reactor core. We take advantage of the equivalence with a nonstandard primal

nonconforming discretization in terms of Hennart's nodal elements by using multi-level iterative solvers designed for nonconforming approximations. Local refinement of the triangulations is realized by an efficient and reliable a posteriori error estimator motivated by a superconvergence result for mixed hybridization. The time-step control relies on extrapolation techniques where the discretization in space is treated as a perturbation of the associated extrapolation tableau.

Numerical results are given for some selected benchmark problems.

AN *HP*-ADAPTIVE BOUNDARY ELEMENT METHOD

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In 1990 the first author developed a successful *hp*-adaptive algorithm for the numerical solution of Symm's integral equation; see [1]. The present work arises from an attempt to extend the methodology of [1] to the boundary integral equations of three-dimensional potential theory. On each surface element, we construct polynomial approximations of maximum degree N using a local basis of products of orthonormal Legendre polynomials; here, $N > 3$ is user specified. The coefficients in these approximations are estimated by collocation and local solution accuracy is measured by the relative size of the higher order coefficients. We present heuristics governing an adaptive solution process in which local polynomial degrees may be increased or decreased and mesh refinement may be implemented in one or both parametric coordinate directions. A number of test problems will be used to demonstrate the effectiveness of the algorithm.

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NONLINEAR BUCKLING ANALYSIS OF 3-D BEAMS BY THE FEM

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The object of this paper is to investigate the effect of prebuckling deflections on the buckling load of beam structures. In [1], Hsiao presented a co-rotational total Lagrangian formulation of beam element for the nonlinear analysis of 3-D beam structures with large rotations but small strains. The internal nodal forces are systematically derived by consistent linearization of the fully geometrically nonlinear beam theory using the virtual work principle. All the terms up to the second order of nodal parameters are retained. Thus, all nonlinear coupling among the bending, twisting, and stretching deformations is considered. The element stiffness matrix is obtained by differentiating the element internal nodal force vector with respect to the nodal parameters, and retaining all the terms up to the first order of nodal parameters. It seems that this element can be applied for the buckling analysis of the 3-D beam structures with the consideration of the prebuckling deflections. Thus, the beam element presented in [1] is employed here.

An incremental-iterative method based on the Newton-Raphson method combined with constant arc length of incremental displacement vector is employed for the solution of the nonlinear equilibrium equation [1]. The zero value of the tangent stiffness matrix determinant of the structure is used as the criterion of the buckling state, and the corresponding load is the buckling load. A bisection method of the arc length is proposed to find the buckling load.

Assume that the equilibrium configuration of the I th incremental step is obtained. Let Δl_I denote the arc length of the incremental displacement vector of the I th incremental step, and λ_I and K_T^I denote loading parameter and tangent stiffness matrix corresponding to the equilibrium configuration of the I th incremental step, respectively. If K_T^{I-1} is positive definite, and K_T^I is not positive definite, the following bisection method is used to obtain the buckling load.

1. Let $\Delta l_L = 0$ and $\Delta l_R = \Delta l_I$; $\lambda_L = \lambda_{I-1}$ and $\lambda_R = \lambda_I$.
2. Let $\Delta l_I = (\Delta l_L + \Delta l_R)/2$. Repeat the I th incremental step to obtain a new λ_I and K_T^I .
3. If K_T^I is positive definite, let $\Delta l_L = \Delta l_I$, and $\lambda_L = \lambda_I$. If K_T^I is not positive definite, let $\Delta l_R = \Delta l_I$, and $\lambda_R = \lambda_I$.
4. Let $\lambda_I = (\lambda_L + \lambda_R)/2$, and go back to step 2.

The above procedure is carried out until a prescribed convergence criterion is satisfied. The buckling load is chosen to be λ_I .

Numerical examples will be presented to investigate the effect of the prebuckling displacements on the buckling load.

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FINITE ELEMENT MODELLING OF PLASTIC DEFORMATION OF MATERIALS WITH PHASE TRANSITIONS

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Considered are axisymmetric problems on martensitic phase transition in a finite volume of a sample of elastoplastic materials. Description of phase transition in elastoplastic materials is based on new thermomechanical criterion [2, 3]. Von Mises isotropic model of elastoplastic deformation is used. Local stresses and strains that are needed for description of phase transition are determined by solving boundary value problem using finite element procedure. The peculiarities of numerical algorithm of solution of above problem are considered. The following problems are studied.

- Appearance of elastic and elastoplastic nucleus with coherent and incoherent interface in a finite volume of a cylindrical sample of elastoplastic materials. The shape of a new phase nucleus (sphere and cylinder) and its position are given as initial data. To take into account of an incoherent interface contact elastoplastic problem is solved [1]. Investigated were conditions of phase transition in a cylindrical and spherical sample at macroscopic compression. The profitability of a new phase nucleation on the sample surface rather than inside of it is shown. It is obtained that incoherent interface considerably changes parameters of phase transition. Effect of superimposed hydrostatic pressure is taking into account analytically.
- Development of plastic strains in elastoplastic compressible sample under cyclic appearance and disappearance of new phase nucleus. It is shown that increments of macroscopic plastic strain per cycle beginning from the second cycle are almost the same.
- Appearance and growth of spherical nucleus of new phase in elastoplastic spherical sample. This problem is solved both analytically and numerically. Studied is the effect of sequence of variation of elastoplastic properties during phase transition on distribution of local stresses and strains.

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ON THE RELIABILITY OF FEM-SOLUTIONS FOR HELMHOLTZ' EQUATION

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The mathematical formulation of scattering and fluid-solid interaction problems is given by variational models based on the Helmholtz equation in an exterior domain or on a system of coupled Helmholtz equations, respectively. The quality of discrete solutions depends on the relation between the physical and geometrical parameters (frequency, domain) and the numerical parameters (stepsize, order of polynomial approximation). In the coupled case, also the relation of material constants fluid/solid is of essential influence. In our talk, we elaborate on the specifics of solution behavior for high frequency and give a survey of our analysis the h - p -Galerkin FEM for Helmholtz' equation. The finite element error is generally polluted. We investigate the dependence of the pollution term on the wavenumber and on the material properties of acoustic media in the coupled problem. We also discuss how the specific error behavior should be taken into account for a reliable methodology of a posteriori error estimation. The theoretical results are complemented by numerical evaluation of model problems.

MODELLING OF ANISOTROPIC MATERIAL BEHAVIOUR FOR THE COMPUTATION OF MAGNETIC FIELDS

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In the recent past some effort has been spent to improve the measurement of anisotropic magnetic behaviour [3]. The measured material data cannot be modelled in a satisfying way using conventional material models, so that the behaviour has to be described using numerical interpolation techniques.

During the computational process the convergence of the non-linear iteration is not always guaranteed. Due to the smoothness requirements of the Newton-Raphson method, the measured data has to be processed to ensure monotonic behaviour of the interpolated $H(B)$ -curves. By applying smoothing techniques on a regularized grid of the interpolated material curves the convergence can be improved. Since the

material curves do not include the saturation region, the saturated behaviour must be extrapolated and the smooth transition between measured data and extrapolated behaviour significantly influences the convergence [2]. Nevertheless it is necessary to apply underrelaxation factors [1] for stabilizing the the Newton-Raphson method.

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PARALLELISING IMPLICIT METHODS ON UNSTRUCTURED GRIDS

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The issue of minimising communication costs whilst maximising computational work is central to the successful parallel implementation of implicit methods. This lecture focuses on the problems which must be addressed to obtain respectable speed-ups on a variety of machine architectures.

The model problem tackled is the solution of a large sparse triangular system of linear equations, typically arising from the ILU decomposition of a matrix resulting from some discretisation of a structural problem. The sequentiality associated with this problem combined with the relatively little computation involved for each variable makes its parallelisation very challenging.

Analysing the directed adjacency graph induced by the triangular matrix yields a unique sequence of *wavefronts* - sets of nodes whose corresponding variables can be computed concurrently. The success of the method depends on the partitioning of the graph between the processors, wavefront by wavefront, so that the work is load-balanced at each step. The difficulty arises in achieving this partition whilst minimising the number of halo nodes between the partitions. Whereas this is, in general, straightforward for a structured mesh, the irregularity of an unstructured mesh can substantially increase the difficulty in achieving a near-optimal partition. Methods for constructing such partitions suitable for both 2D and 3D grids are presented.

For many machines, the latency cost incurred between each each wavefront is prohibitively expensive and so reduction in the number of wavefronts, whilst sacrificing

some of the parallel workload, is required for speed-up to be achieved. The compromise between maximising parallel computation and minimising communication must be flexible in order for the method to be applicable to a wide range of parallel machines and this is facilitated by the use of a cost model.

The BSP (Bulk Synchronous Parallel) parallel model [1] (L.G.Valiant, W.F.McColl) was designed as a unifying abstraction of a general-purpose parallel computer. The components of a BSP computer are

- a set of sequential processors with local memory
- a communication system which processors can use to access non-local data
- a mechanism for globally synchronising the processors

The quantitative differences between machines due to network topology, for example, are reflected within the model by parameters defining the cost of accessing data in remote memory. The BSP model constitutes a *uniform* cost model for remote memory access and, thus, the assumption is that the time to fetch a remote data item does not depend on its location. The processors of a BSP computer proceed through a series of *supersteps*, globally synchronising after every superstep. A superstep consists of a segment of computation and can contain requests to fetch from or store to remote processors; the requests for data are guaranteed to have taken place by the start of the next superstep. The BSP hardware model, therefore, can be parametrised by

- p = number of processors
- s = processor speed
- L = barrier synchronisation time
- g = ratio of total CPU capacity to total communication capacity

The values of L and g are likely to depend on p .

The BSP library [2], [3] is an implementation of the model and enables code portability together with efficient inter-processor communication amongst a variety of hardware architectures. Accurate predictions of the execution time of a BSP program can be made using the model by estimating the maximum computation at each superstep and the maximum communication between each superstep. The model can, therefore, be incorporated into a partitioning algorithm resulting in partitions best suited to their target machines.

The Oxford BSP library is used to implement the parallel triangular solver and results compare favourably against shared-memory directives on the Silicon Graphics' Power Challenge.

The incorporation of this method into a CG solver with ILU preconditioner is described with corresponding results on the Silicon Graphics' Power Challenge and the IBM SP2. Whereas, recently, the block ILU CG method has received much attention due to its low communication requirements (resulting in slower convergence), we show that good speed-ups can be obtained whilst retaining the original convergence rate. Increasing the workload per grid node can further improve the speed-up, making this a feasible parallel solver for even distributed-memory machines with high communication costs.

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A VISCOELASTIC HIGHER-ORDER BEAM FINITE ELEMENT

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The viscoelastic internal variable constitutive theory of Johnson, et al. [2, 1] is applied to the higher-order elastic beam theory and finite element formulation of Tessler [3]. The viscous material in the beam is approximated by a discrete internal Maxwell solid. The viscous finite element formulation has additional sets of nodal variables for each time constant needed in the discrete Maxwell solid. Recent developments in modeling viscoelastic material behavior with strain variables that are conjugate to the elastic strain measures are combined with the advances in the modeling of through-the-thickness stresses and strains in thick beams. The result is a viscous thick-beam finite element that possesses superior characteristics since the viscous forces do not suffer from linear dependency on the nodal velocities, which is the case when damping matrices are used. Instead, the viscous forces are directly dependent on the material's relaxation spectrum and how it relates to the nodal variable velocities. The thick beam analysis is explored herein as a first step towards developing more complex viscoelastic models for thick plates and shells.

The internal variable constitutive theory is derived directly from the Boltzmann superposition theorem. The mechanical strains and the internal strains are shown to be connected by a system of first-order ordinary differential equations. The total time-dependent stress is the superposition of the elastic and viscous components of stress. Equations of motion for the solid are derived from the virtual work principle using the total time-dependent stress. Computational examples are carried out for viscoelastic beams made from a material with a complicated Maxwell model.

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COMPARISON OF DATA PARTITIONING AND DOMAIN DECOMPOSITION METHODS IN REAL LIFE PROBLEMS

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In the field of partial differential equations, data partitioning and domain decomposition methods belong to the most effective parallelization techniques.

A direct parallelization leads to so called data or grid partitioning strategies. The parallel version shows the same algorithmic behavior as the serial one but suffers from a sometimes considerable communication overhead. This disadvantage has led to indirect parallelization strategies (e.g. accelerated Schwarz methods) which are characterized by an additional outer iteration.

In [1] an overview of the above methods was given, and their performance were compared in our *industrial simulators*. Here we present performance results for selected real life examples from

- fabrication of semiconductor devices
- nuclear reactor analysis
- simulation of electric circuits in time domain

both for a workstation network and for a multi processor shared memory architecture. In process simulation of semiconductor devices as well as in nuclear reactor analysis, nonlinear partial differential equations of parabolic type have to be solved. In process simulation, direct parallelization methods, i.e. parallel multigrid in connection with Newton's method and parallel CGS, turn out to be superior to indirect ones. Even for a workstation cluster (12 SUN-Sparc2), a speed up of more than 7 has been achieved for point defect simulation.

The modelling of electric circuits leads to large systems of differential algebraic equations. Due to an unstructured Jacobian, direct solvers have to be used. Thus, direct parallelization leads to Schur complement methods, which suffer from a communication overhead. Here, indirect methods in terms of the multi level Newton method seem to be the better choice. On a 8 processor SGI Power Challenge, speed up results of 5 are achieved.

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RECIPROCITY FORMULATIONS FOR REGULAR BOUNDARY ELEMENT AND FINITE ELEMENT METHODS

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For simplicity the formulation steps for Poisson's differential equation in two dimensions are presented, despite the presented method is not restricted to that. The full paper includes regular boundary element (RBE) formulation and the technique how the formulation is used to obtain finite element (FEM) scheme. The treated problem governed by the Poisson's equation with given domain and boundary: It can be written as

$$\nabla^2(u) = b(x, y).$$

The boundary values are mixed i.e. natural or essential boundary values are prescribed over the parts of boundary. In the case of weighted residual formulation one can use the solutions to the homogeneous version of the governing (Laplace's) equation as weighting functions. For achieving boundary integral equation reciprocity formulation is made, i.e. the equation is multiplied by the weight function and integrated by parts twice. In the resulted integral equation there is still one domain term which is also transformed by reciprocity principle. For doing that the domain source or inhomogeneity is approximated by an expansion of functions which are invariant to Laplace's operation. Such families of functions are easily produced. They are analogous to the usual FEM interpolation functions. The expansion uses as many unknown multipliers as the number of unknown problem values are. One has N boundary and L domain values to produce. The technique is actually a new version of dual reciprocity formulation utilised widely in BEM. The formulation results in a number of integral expressions. This number is equal to the number of weight functions used. The simplest way of producing the necessary number of weight functions is the usage of boundary and domain (collocation) nodes as 'source' points of the functions. When the integral formulation finished, the matrix formulation is made by dividing the boundary into elements and applying the integral statements. The domain is also treated by point or subdomain collocation. In the latter case the domain is also divided into elements. The numerical (matrix) formulation results in an equation of type

$$Hu - Gq = (HU' - GQ')F^{-1}b$$

Where upper case letters are system matrices, u , q and b stand for problem variable, its outward normal derivative and the domain source, respectively. F (and its inverse) contains only values completely determined by the "interpolation" functions and can be different according to the domain approximation technique. In the paper point and subdomain collocation are implied. All the other system matrices are formulated by the usual boundary element discretisation. Their forms depend on the order

of approximation over the elements. After applying the boundary conditions and rearranging the matrix equation, a linear system of equation is produced. In the case of point collocation a boundary element scheme is established with unknowns also in the domain collocation points. However if one uses domain discretisation with subdomain collocation over the elements, a finite element system is resulted with no explicit assemblage but the system matrix will be fully populated. To produce a sparse matrix equation (6) should be used to small (finite) elements with some nodes when formulation is followed by assembling the system matrix. A third basic possibility is the establishment the method of subdomains, when equation (6) is applied to subdomains which are then assembled. In the paper formulation for different element types are described and compared. A more general comparison is also made including RBEM and the different FE formulations. The paper presents the outlined methods through simple two dimensional examples. A survey on more complex 3D and time dependent problems is also given. The application of the method to diffusion, heat transfer and elasticity problems is also discussed briefly.

FINITE ELEMENT APPROXIMATION FOR 2ND ORDER ELLIPTIC EIGENVALUE PROBLEMS IN MULTI-COMPONENT DOMAINS WITH NONLOCAL ROBIN TRANSITION CONDITIONS AT THE INTERFACES

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In this paper we deal with a finite element method for an elliptic eigenvalue problem in a multi-component structure in 2D, with nonlocal Robin-type transition conditions at the interface. To fix the ideas, let Ω be a rectangle, divided by the line Γ into two rectangles Ω_1 and Ω_2 , and consider the following eigenvalue problem (EVP): find $[\lambda, u^1, u^2] \in \mathbf{R} \times H^2(\Omega_1) \times H^2(\Omega_2)$, which obey, in a weak sense, the pair of differential equations

$$-\operatorname{div}(k^1 \cdot \operatorname{grad} u^1) + a_0^1 u^1 = \lambda u^1, \quad \text{in } \Omega_1, \quad (1)$$

$$-\operatorname{div}(k^2 \cdot \operatorname{grad} u^2) + a_0^2 u^2 = \lambda u^2, \quad \text{in } \Omega_2, \quad (2)$$

together with the transition conditions

$$-k^1 \frac{\partial u^1}{\partial n} = h^1(u^1 - F(u)), \quad \text{on } \Gamma, \quad (3)$$

$$-k^2 \frac{\partial u^2}{\partial n} = h^2(u^2 - F(u)), \quad \text{on } \Gamma, \quad (4)$$

as well as with homogeneous Neumann boundary conditions on $\partial\Omega_1 \setminus \Gamma$ and $\partial\Omega_2 \setminus \Gamma$.

Here,

$$F(u) = C \int_{\Gamma} (h^1 u^1 + h^2 u^2) ds, \quad (5)$$

and h^1, h^2, a_0^1, a_0^2 are sufficiently smooth given functions, while C is constant.

The problem arises in the context of some heat transfer problems in buildings.

By passing to a proper variational formulation in a product Sobolev space setting, we show that the present type of EVP can be put into the framework of abstract elliptic eigenvalue problems in Hilbert spaces, for bounded, symmetric and coercive bilinear forms, as studied in well-known references as e.g. Raviart and Thomas.

We consider finite element methods with and without numerical quadrature and discuss the involved error estimates.

VISCOUS FLOWS NEAR BOUNDARY SINGULARITIES

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It is well known that the presence of one or more boundary singularities affects adversely the convergence, with decreasing mesh- or element-size, of the numerical solution of boundary value problems (BVPs). In this context, the accurate simulation of viscous flow phenomena in the neighbourhood of sharp corners presents a rich and varied challenge to numerical methods, and integral-equation methods have proved eminently suitable, particularly in Stokes flow problems, in this light.

An overview will be presented of the author's work in this field, specifically in:

- *singularity subtraction* (SS) methods, in which the entire BVP must be pre-processed in order to solve for a regular function which is post-processed to recover the required physical solution;
- *singularity incorporation* (SI) methods, which use physical information except in a neighbourhood local to the singularity, thereby minimising the need for pre-processing;
- *singularity annihilation* (SA) methods, recently developed by the author, in which no pre-processing at all is required, merely a judicious choice of Green's function in the integral formulation.

The pros and cons of each method will be briefly addressed, and results of the application of all three approaches to viscous flow problems will be presented.

ALGORITHMS FOR CONTACT PROBLEM WITH FRICTION IN THERMOELASTICITY

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We draw on the mathematical formulation of the Contact Problem, which leads to the seeking of the saddle point of the Lagrangian $\mathcal{H}(\mathbf{v}, \mu)$ over the set of admissible displacements K and the set of admissible multipliers Λ , where

$$\mathcal{H}(\mathbf{v}, \mu) = \frac{1}{2}A(\mathbf{v}, \mathbf{v}) - L(\mathbf{v}) + j(\mathbf{v}, \mu) \quad ,$$

$$K \equiv \{\mathbf{v} \in V \mid v'_n - v''_n \leq 0 \text{ on } \Gamma_c\} \text{ and } \Lambda \equiv \{\mu \in L^2(\Gamma_c) \mid |\mu| \leq 1 \text{ on } \Gamma_c\}$$

and V is the space of virtual displacements.

This formulation enables additional contact elements to be avoided, where a suitable stiffness parameter is needed. Moreover, we obtain the asymptotic estimate of the error of an approximate solution. Discretization then leads to the sequence of the following Quadratic Programming problems:

$$f(x) = \frac{1}{2}x^T Cx - x^T d \rightarrow \min$$

with constraints

$$Ax \leq 0.$$

Therefore, we can examine a great variety of methods and select the optimal in view of the speed and memory requirements. Particularly, we test The Conjugate Gradient Method (with projected gradient) and its modifications, including various preconditioners. The methods based on the elimination are discussed as well.

The geodynamical model is analysed in the application. It simulates the motion of lithospheric plates in the Earth and can be regarded as a quasistatic study of a dynamic tectonic plate model which mathematically describes the collision zones in the sense of new global tectonics.

A NUMERICAL STABILITY OF THE FE SOLUTION OF MAXWELL'S EQUATIONS IN THE TIME DOMAIN

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A method is described to derive finite element schemes for the electromagnetic waves propagation in free space in one or more space dimensions. The governing equations are Maxwell's equations

$$\epsilon_0(\partial \mathbf{E}^* / \partial t) = \text{curl } \mathbf{H}^*, \quad \mu_0(\partial \mathbf{H}^* / \partial t) = -\text{curl } \mathbf{E}^* ,$$

which are expressed in a conservation form

$$\partial \mathbf{U}^* / \partial t + \partial \mathbf{F}_j^* / \partial x_j = 0, \quad j = 1, 2, 3 ,$$

where the summation convention has been employed and where $\mathbf{U}^* = [\mathbf{E}^*, \mathbf{H}^*]^T$.

To produce accurate differencing, the method employs forward-time Taylor series expansions including time derivative of second and third order

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \Delta t \partial \mathbf{U} / \partial t |^n + (\Delta t^2 / 2) \partial^2 \mathbf{U} / \partial t^2 |^n + (\Delta t^3 / 6) \partial^3 \mathbf{U} / \partial t^3 |^n .$$

This yields a generalized time-discretized equation which is successively discretized in space by means of the standard Euler-Taylor-Galerkin finite element method.

The technique is illustrated first in one space dimension with linear and quadratic elements using the implicit (consistent) and explicit (diagonal) numerical schemes. To analyse the properties of the Euler-Taylor-Galerkin finite element scheme we substitute a Fourier mode $\exp ikz$ into it and find e.g. for linear elements and time derivative of second order the amplifications in one time step of

$$\lambda_{1,2}(p) = 1 + [1/3(\cos p + 2)]^{-1}[\pm iC \sin p - 2C^2 \sin^2 1/2p]$$

which, in the asymptotic limit $p \rightarrow 0$, reduces to

$$\lambda_{1,2}(p) \approx 1 \pm iCp - 1/2C^2p^2 + O(p^3)$$

to be compared with $\exp iCp$ for the system of differential equations. It follows that the Euler-Taylor-Galerkin finite element scheme is the second-order accurate. The stability CFL-type condition reads $C < \sqrt{3}/3$ for $|\lambda_{1,2}(p)| \leq 1$.

This method applies to initial value problems with periodic data. It is of practical interest that the von Neumann approach always yields a necessary condition for stability and in many cases this is also a sufficient condition. A study of improving the stability properties to deal with higher order elements and higher order terms of Taylor series expansion for the time domain is discussed.

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FINITE ELEMENT SOLUTION OF SEMIDISCRETIZED PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS WITH NON-SMOOTH INITIAL DATA

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A-stable methods combined with finite element Galerkin discretization of spatial variables, often result in loss of accuracy for the numerical solution of parabolic equations with high frequency components in the solution or with irregularities in initial-boundary conditions. L-stable methods combined with finite element Galerkin approach for the spatial variables are presented. The methods have the property to damp high frequency components in the solution with no restriction on time and space steps, unlike A-stable methods. The methods developed are based on rational functions with real and distinct poles. Parallelism is achieved by utilizing partial fraction decomposition of rational functions with matrix arguments, thereby allowing the distribution of work in solving the corresponding linear algebraic systems in essentially Backward Euler-like solves on concurrent processors. Numerical results are presented.

THE COMPLETE ASSEMBLAGE OF LET SHAPE FUNCTIONS FOR THE FINITE ELEMENT METHOD

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This paper presents results of analytical construction of the complete assemblage of Linearly - Exponentially - Trigonometrical (LET) shape functions for an arbitrary number of boundary nodes for rectangular finite elements. The set of LET shape functions is complete with respect to the set of nodes used.

In contrast to traditional FEM the nonpolynomial shape functions satisfy to the governing equations and can be found in explicit analytical form for an arbitrary number of boundary nodes.

The algorithm for construction the shape functions constructed on the base the law of boundary superposition, method of lines and the finite functional Fourier series.

In limit case (when number of nodes tends to infinity) the shape functions tends to components of boundary Green's function. For the first time classic solution of Dirichlet's problem for rectangular parallelepiped is given.

For problems of the plane elasticity is used the schemes of compound integration. Optimization of computational process is given. For problems of bending of very thin plates presents new nonlocking finite element schemes of numerical integration.

The main reason of locking is that, stiffening effects are introduced by the cor-

ner's bilinear terms in shape functions. At this reason the stiffness matrix of shear presents in form of sum of four terms: bilinear, two mixed and nonpolynomial. For everyone term of shear stiffness matrix is used own integration. For example, for a bilinear term shear energy coefficients are evaluated using one-point quadrature while the nonpolynomial terms are evaluated using the usual four-point (two in each coordinate direction) quadrature. Numerical results demonstrate that this LET-element is effectively free of locking even for very thin plates.

BIFURCATION AND CHAOS IN TIME-INTEGRATION SCHEMES FOR SPATIALLY DISCRETIZED FIELD EQUATIONS

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Consider the following system of second-order nonlinear ordinary differential equation:

$$\mathbf{M}\ddot{\mathbf{x}} + \mathbf{p}(\mathbf{x}, \dot{\mathbf{x}}) = \mathbf{f}, \quad (1)$$

where \mathbf{p} is a nonlinear algebraic function of displacement \mathbf{x} and velocity $\dot{\mathbf{x}}$. This equation might be the equation of motion of a nonlinear elastic or viscoelastic system. If we consider the case when \mathbf{f} is the vector of external forces, \mathbf{M} is the mass matrix and $\mathbf{S} = \partial \mathbf{p} / \partial \mathbf{x}$, $\mathbf{D} = \partial \mathbf{p} / \partial \dot{\mathbf{x}}$ are stiffness and damping matrices, respectively, equation (1) represents obviously the semi-discretized equation of motion by finite elements of a viscoelastic structural problem.

Completing the above equation with initial conditions the solution requires in general a step-by-step numerical time-integration procedure. In the case of a nonlinear heat conduction problem, the semi-discretization by finite elements leads to the following field equation:

$$\mathbf{C}\dot{\mathbf{x}} + \mathbf{k}(\mathbf{x}) = \mathbf{f}, \quad (2)$$

where \mathbf{x} is the vector of nodal temperatures, \mathbf{C} is the heat capacity matrix and $\mathbf{K} = \partial \mathbf{k} / \partial \mathbf{x}$ is the conductivity matrix.

The aim of this paper is to study instable and chaotic behavior of solutions appearing in some finite-difference schemes. Our interest is in the change of dynamic behavior of solutions of equations (1) and (2) when the time-step as bifurcation parameter changes. It must be emphasized that it is almost impossible to estimate a priori at what value of the time-step there appear instabilities or chaotic response. Hence, the following question is naturally posed: how could we ensure the unconditionally stable response independently of the time-step selected. The importance of the question lies therein that in most commercial finite element codes the simplest schemes (e.g. Newmark- β , Wilson- Θ , etc.) are used and these methods exhibit the worst chaotic behavior when applied in nonlinear problems. In order to demonstrate these effects, a single degree-of-freedom, unforced, undamped dynamical system as special case of eq. (1) has been chosen.

STABILITY OF MULTILAYERED RINGS

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In this paper the critical load of multilayered rings is determined in case of dead load and hydrostatic load. The ring contains arbitrary number of soft and hard layers, where the soft layers are compressible in normal direction. In the hard layers it is supposed that the Bernoulli- hypothesis is valid and for the soft layers the sections normal to the mid- plane are supposed to remain plane after the deformation. The governing differential equation is derived by using a variational principle. The critical load is determined applying the method of successive approximation. The obtained results are compared with the numerical results of finite element computations in the COSMOS/M program system. During the development of the finite element model, different model building strategies were compared and for the calculations the most efficient one is used. As conclusion we can say that the finite element and approximate results are in a good agreement. The results obtained here can be useful during the experimental test program for multilayered beams. This project is sponsored by the Hungarian Foundation for Scientific Research (OTKA) in the frames of the research project OTKA T-4406.

HIERARCHICAL STRUCTURAL MODELLING WITH A COMBINATION OF *H*- AND *P*-VERSION FINITE ELEMENTS

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An engineering design process is in a natural way a hierarchical procedure. First a draft of the most suitable structure is chosen from a variety of alternatives, by the criteria of some global structural properties, avoiding all unnecessary details. This coarse model is then refined in a sequence of design levels, and in each step a new model is constructed with loads and boundary conditions being estimated from the results of the previous step. Because each design level is represented by a new computation with specific analysis data, the problem rises to transport the necessary information between the isolated levels. This procedure is time consuming and numerically unsatisfying.

In this work, an approach for a hierarchical structural design is presented. Due to a multi-scale finite element procedure, the method implicitly enables the reuse of all information, obtained in all levels of the model. In our formulation, an *hp*-domain decomposition algorithm is constructed, using *p*-version elements to model

the global behavior of a structure. An adaptive h -version is used in sub-domains, where detailed information of the solution, e.g. local stress at joints, is needed. The h -version finite element mesh can be simply overlaid the p -version model, thus representing a hierarchical enrichment of the approximation space.

It will be outlined, that the computations on both length-scales can be performed independently, so that standard error analysis is directly applicable. Both computations are coupled through strains and prestrains in an iterative procedure. Furthermore, assuming the same strain measure on the interface of the local and global model, different types of analysis can be used on each scale.

Our paper shows the algorithmic background of this method and presents as a numerical example a steel frame of a fabrication hall with midrange cranes, being typical for this kind of multi-scale design problems. Due to the large displacement of the global structure, the nonlinear behavior of the frame is analyzed by a p -version finite elasticity method. The console, where accurate stresses are necessary for a fatigue computation, is represented by an adaptive h -version.

ON THE 2D AND 3D FEM PRE- AND POST-PROCESSING

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In the contribution the idea of the pre- and post-processing for the two and three dimensional finite element mesh will be discussed.

The pre-processing consists of generation of the finite element mesh. This is based on modified Delaunay-Voronoi method and utilizes certain relaxation techniques to improve the final quality of the generated mesh.

The post-processing includes several methods for data visualization as slicing, isosurfacing and direct volume rendering, which enable direct visual survey of the results of any FEM computation.

Problems from geodynamics will be presented and use of the above methods shown.

AN ANALYSIS OF FINITE ELEMENT VARIATIONAL CRIMES FOR A NONLINEAR ELLIPTIC PROBLEM OF A NONMONOTONE TYPE

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In practical implementation of the finite element method to boundary value problems, the so-called *variational crimes* are usually committed: the given domain with a piecewise curved boundary is approximated by a polygonal (in $2d$) or polyhedral (in $3d$) domain and integrals are evaluated approximately with the use of numerical quadratures. The theory of finite element variational crimes for linear problems was extensively studied, e.g., by Ciarlet, Raviart, Strang in seventies. A detailed analysis of various nonlinear problems was later given by Berger, Feistauer, Sobotíková, Ženíšek, etc.

However, not all types of nonlinear equations important in practice are covered in papers of the above mentioned authors. We shall be concerned with finite element approximations of the quasilinear equation

$$-\nabla \cdot (A(x, u) \nabla u) = f(x)$$

in a bounded domain $\Omega \subset R^d$, $d \in \{1, 2, \dots\}$, with Dirichlet boundary conditions. We assume that Ω has a Lipschitz-continuous boundary and that $A = (A_{ij})_{i,j=1}^d$ is a smooth and uniformly positive definite matrix with respect to all variables. It is easy to prove that the above problem is nonpotential and does not lead to a problem with a monotone operator, in general.

Moreover, the well-known Kirchhoff transformation cannot be applied in the case of anisotropic nonlinear media (for instance, in examining a temperature field in the magnetic circuit of a transformer, where nonlinear temperature dependencies of heat conductivities along and across lamination differ, i.e., $A_{11} \neq A_{22} = A_{33}$).

We will employ a general quadrature formulae and prove the existence of approximate finite element solutions. Furthermore, we examine their convergence to the true solution u in the H^1 -norm without any regularity assumption upon u .

METAL FORMING SIMULATION - A CHALLENGE FOR FEM ANALYSTS AND SOFTWARE DEVELOPERS

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Although tool and process design for metal forming operations is a very difficult job, predictive simulation tools like finite element process simulation have not really been accepted by the tool designers in the past; time consuming analyses for more or less academic applications caused by inadequate finite element formulations and program architectures, severe mesh distortion and contact problems made it impossible to perform "real-world" forming simulation. In the meantime there are a few specialized or multi-purpose FEM codes available, which meet the demands of design engineers to some extent.

Consistent integration algorithms for the constitutive equations, robust element models, flexible contact algorithms, fully automatic remeshing strategies, fast equation solvers and last but not least the increase of computer speed paired with the decrease of hardware cost are only a few catchwords to point out the major areas of progress.

The paper will try to give an overview over the state of the art in the fields of sheet and bulk metal forming analysis. Examples of typical industrial applications will be presented to demonstrate contemporary capacity of metal forming simulation. Still existing shortcomings of FEM technology from the point of view of practical application and efficiency will be shown and the need for further developments will be summarized.

A MATHEMATICAL MODEL FOR A CLASS OF HYSTERESIS PROBLEMS

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Stress-induced martensitic transformations in shape memory alloys exhibit hysteretic behaviour, i.e. in the course of a loading/unloading process there is a hysteresis loop in load-deformation space. This interesting phenomenon was recently investigated both experimentally and in the framework of irreversible thermodynamics by I. Müller and his coworkers, who introduced a concept of ideal pseudoelasticity. Further thermodynamical explanations of the dissipative, pseudoelastic behaviour were proposed by V.I. Levitas. It should be noted that a free energy function of the two-phase solid mixture is nonconvex.

In this talk our aim is to present a useful, compact mathematical description for pseudoelastic problems. We set the dissipative problem in the framework of evolutionary variational inequalities with a jumping parameter, taking advantage of some similarity which exists between the pseudoelastic behaviour and the elastoplastic one. The finite element solution of the incremental problem is determined by solving a complementarity problem. Numerical results for test problems are given.

NUMERICAL ASPECTS OF THE INEQUALITY PROBLEMS FOR STRUCTURES ON FOUNDATIONS

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We are concerned with the inequality problem for a plate resting on a foundation. The unilateral interaction conditions between the plate and its foundation are taken into account. For the plate the kinematical model of Reissner-Mindlin is applied and the elasto-plastic material behaviour is supposed. The foundation is modelled as an elastoplastic medium of Winkler type. These fundamental assumptions impose inequality constraints on some quantities describing the plate-foundation system and, on the mathematical side, lead to a unilateral boundary value problem. We present a unified approach to this problem in which both the conditions of unilateral contact and those of elasto-plastic behaviour are governed by variational inequalities. Computational aspects of the finite element solution of the weak formulation of this inequality problem, which consists of a variational equation and three variational inequalities, are discussed. The grillage analogy is employed for the finite element discretization of the plate, with linear grillage elements exhibiting no shear locking effects. The incremental discretized problem under consideration is solved as a complementarity problem. Numerical results for test problems are provided.

ANISOTROPIC ERROR ESTIMATORS FOR SIMPLICIAL FINITE ELEMENT MESHES

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Some boundary value problems yield anisotropic solutions, e.g. solutions with boundary layers. If such problems are to be solved with the finite element method, anisotropically refined meshes can be advantageous. In order to construct these meshes or to control the error one aims at reliable error estimators.

Our investigations are restricted to the Poisson equation

$$-\Delta u = f \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial\Gamma_D = \partial\Omega$$

in a polygonal domain Ω . Some basic difficulties arising from the anisotropy are reflected here sufficiently well.

For isotropic meshes residual error estimators for a finite element T are well known:

$$\eta_T(u_h) := \left(h_T^2 \cdot \|f\|_T^2 + \sum_{E \in \partial T \setminus \Gamma_D} h_T \cdot \|r_E(u_h)\|_E^2 \right)^{1/2}.$$

Here u_h is the approximate solution, h_T is the diameter of T , and $r_E(u_h)$ is the gradient jump across an internal face E . All norms are L_2 norms. With this notation

$$\|\nabla(u - u_h)\|^2 \leq c \cdot \sum_{T \in \mathcal{T}} \eta_T^2(u_h) \quad (1)$$

holds.

For problems with an anisotropic solution (eg. a boundary layer) one may use anisotropic meshes, i.e. meshes where the aspect ratio of the elements can be very large. Then the constant in (1) becomes large, and the estimation is unsatisfactory.

This behaviour can be remedied by anisotropic error estimators. Siebert investigated this for cuboidal meshes. Here we focus on simplicial meshes and obtain the estimator

$$\eta_{1,T}(u_h) := \left(h_{min,T}^2 \cdot \|f\|_T^2 + \sum_{E \in \partial T \setminus \Gamma_D} h_E \cdot \|r_E(u_h)\|_E^2 \right)^{1/2} \quad (2)$$

where the factors of the norms are replaced by the smallest element size $h_{min,T}$ and the height over the h_E the face E , respectively.

Recently also an L_2 error estimator for anisotropic meshes could be derived.

A main difference to isotropic error estimators is that the anisotropic problem and the anisotropic mesh have to correspond in some way. This is reflected by several assumptions that are required for the proofs of the estimations.

EXTRACTION OF FINITE ELEMENT RESULTS BASED ON VIRTUAL WORK

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In many applications the primary aim of a finite element analysis is to obtain few design quantities with a prescribed accuracy. In structural mechanics quantities such as surface forces and surface force densities (hereafter denoted surface tractions) are often important for design decisions. Thus in such cases the quality control of the numerical results need to be performed on these quantities. This includes both control of the qualitative and quantitative behavior of the computed results.

In this paper, a general concept for recovery of surface forces and surface tractions which makes use of the principle of virtual work is presented. The novelty of the presented approach lies in the way virtual work consistent element boundary tractions are used to make the recovery technique applicable without imposing *a priori* restrictions on the mesh.

An important qualitative feature with the presented technique is that static equilibrium between recovered surface forces or surface tractions and the applied forces is always satisfied. Surface forces or surface tractions obtained directly from the finite element stress field derived through differentiation of the finite element displacements do not satisfy this important qualitative feature.

First the theoretical aspects are addressed, including the definition of virtual work consistent element boundary tractions. Then an outline of how the presented concept for extraction of finite element results can be utilized to recovery of surface forces and surface tractions are given. A numerical example that illustrates the obtained accuracy in the computed surface tractions are provided for a plane stress problem.

THE PANEL CLUSTERING ALGORITHM FOR PETROV-GALERKIN DISCRETISATIONS

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In 1986 Hackbusch and Nowak developed the panel clustering algorithm to reduce the computational work and the storage requirements of the collocation method. The algorithm constructs an approximation B^{pc} of the system matrix B described by the splitting

$$B^{pc} := B^{near} + B^{far} U^{far},$$

where the near field part, B^{near} , is a sparse matrix with $\mathcal{O}(n)$ nontrivial entries (n denotes the number of unknowns).

In the talk we present a formulation of the panel clustering algorithm valid for all Petrov-Galerkin discretisations. Considering a $(d - 1)$ -dimensional boundary the far field part, i.e. the matrices B^{far} and U^{far} , can be computed by $\mathcal{O}(n \log^{2d+1} n)$ operations to get an approximation sufficiently close to B . The storage requirements amount to $\mathcal{O}(n \log^{d+1} n)$. In the special case of the collocation method the computational work can be reduced to $\mathcal{O}(n \log^{d+2} n)$.

This formulation of the algorithm leads to an efficient and flexible implementation that enables us to consider panel clustering as 'black box accelerator'. Some numerical examples will be given.

FINITE ELEMENT METHODS FOR STATIONARY AND STATIC FIELD COMPUTATIONS

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In our talk we shall present a finite element method for computing stationary and static electromagnetic fields directly in terms of the electric and magnetic field strengths. As compared to the classical finite element formulation in terms of (vector) potentials our method has the advantage that the accuracy with which the field strength is computed is one order higher. Further, unlike potential based methods, the direct computation of the field strength does not require gauging.

The formulation we use requires a discretization technique that allows the modelling of continuity conditions for the field at interfaces between media with different electric and/or magnetic properties. To this end, a combination of nodal and edge expansion functions is employed, using edge expansion functions for modelling the field along discontinuities and nodal expansion functions in homogeneous subdomains. Edge expansion functions are also used on slanted parts of the outer boundary and near reentrant corners.

As compared to time- and frequency-domain formulations, the computation of the electromagnetic field in the stationary and static states has certain characteristics. Firstly, the compatibility relations need to be made explicitly a part of the formulation in order to ensure the uniqueness of the solution. Secondly, the well known decoupling of the electric and magnetic fields requires that the stationary magnetic, stationary electric and electrostatic fields need to be examined separately. These three cases can, however, be combined in one generic formalism.

The above ideas were implemented in the finite element code FEMAXS for computing fields in inhomogeneous, (an)isotropic and (non)linear media.

The accuracy of the proposed method is illustrated by solving a boundary value problem with a known analytical solution, the so-called "semi-infinite gap" recording head configuration [1].

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MULTILEVEL FINITE ELEMENT METHODS IN CHEMICAL COMPUTING

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Large chemical process simulation represents a class of challenging problems. The development of robust and highly efficient codes has been a topic of continuing investigations during the last years.

For solutions possessing sharp moving spatial transitions as travelling wavefronts or emerging boundary and internal layers, an automatic adjustment of both the space and the time step is generally accepted to be more successful in efficiently resolving critical regions of high spatial and temporal activity. Consequently the solutions are as accurate as required by the user and the necessary work to obtain such solutions is minimized.

The lecture will survey some of the essential features of such adaptive methods, which have been developed recently by the author. Real-life chemical problems are inserted to illustrate the relative merits of the proposed method implemented in the program package KARDOS.

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ADAPTIVE FINITE ELEMENT APPROXIMATIONS FOR NONLINEAR PARABOLIC SYSTEMS

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A large number of phenomena in biology, ecology, physics and engineering is set up by time-dependent systems of PDEs of the following type

$$H(x, t, u)u_t - \nabla \cdot (D(x, t, u)\nabla u) = F(x, t, u, \nabla u) \\ x \in \Omega \subset \mathbb{R}^n, t > 0, n = 1, 2$$

where additional boundary and initial conditions are included. The heat capacity matrix H and the diffusion matrix D may be singular, the right-hand side vector F describes some coupling of the components and allows to take into account mild convection.

Adaptive computations of those equations play an increasingly important role in dynamical process simulation. The efficient adaptation of the spatial and temporal discretization is often the only way to get relevant solutions of the underlying mathematical models. In our lecture fully adaptive solutions of nonlinear parabolic equations in 1D and 2D employing the discretization sequence first in time then in space are presented. The time discretization is done by a singly diagonally implicit Runge-Kutta method (SDIRK) controlled by an embedding strategy. A posteriori error estimates for the finite element discretization in space are obtained by solving local linear elliptic problems with higher accuracy. Once those estimates have been computed, we are able to control time and space grids with respect to required tolerances and necessary computational work.

We shall discuss in detail the construction of the selfadaptive time-space finite element method. Furthermore, the corresponding error estimations which are a central part of the proposed method are focussed on. We report results for real-life problems.

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ADAPTIVE DOMAIN DECOMPOSITION METHODS IN FEM AND BEM

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Nowadays Finite Element (FE) and Boundary Element (BE) Galerkin methods are widely used for solving Partial Differential Equations (PDE) numerically. In many practical applications, the use of the FEM and of the BEM in different subdomains of a non-overlapping Domain Decomposition (DD) and their coupling over the coupling boundaries (interfaces) brings about several advantages. For instance, in the magnetic field computation for electric motors, we can use the BEM in the air subdomains including the exterior of the motor more successfully than the FEM which is preferred in ferromagnetic materials where non-linearities can occur in the PDE, or in subdomains where the right-hand side does not vanish. The same is true for many problems in solid mechanics. The non-overlapping DD is a powerful tool not only for coupling FEM and BEM but also for the construction of highly efficient parallel solvers for the large-scale systems arising.

The paper is mainly concerned with the design, the analysis and the implementation of fast and well adapted parallel DD solvers for large-scale FE-, BE- and coupled FE/BE-equations approximating magnetic field problems and linear elasticity problems. The solvers developed are of asymptotically optimal, or at least almost optimal algebraic complexity and of high parallel efficiency. The domain decomposition as a technique for data partitioning, structuring and mapping onto a topology of processors is a difficult procedure for real-life problems. Thus, we develop the tool **ADDP** for the automatization of the domain decomposition procedure taking into account data properties (material properties, properties of the right-hand side, boundary conditions etc.) as well as the expected complexity of the local problems arising (load balance problem !). The theoretical analysis is substantiated by a lot of numerical results obtained by the code **FEM \otimes BEM** on various massively parallel machines with up to 128 processors.

NUMERICAL AND EXPERIMENTAL INVESTIGATION OF THE MECHANICAL BEHAVIOUR OF FIBRE REINFORCED MULTILUMIC PRESSURE HOSES

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The mechanical behaviour of fibre reinforced multilumic pressure hoses essential depends on the twist angle of the fibre structure. An unsymmetrical cross-section gives the possibility of pressure controlled deflection, which is the basis for the development of very thin flexible endoscopes for minimally invasive neurosurgical techniques. In the paper the theoretical basis for the numerical simulation and optimization of fibre reinforced hoses is given. For the analysis of this geometrical and physical non-linear problem a special FEM-code has been developed. For the solution of large displacements the Update-Lagrangian Formulation is used. The truss elements are coupled with three-dimensional solid elements using the Penalty Function Methode. To simulate different material properties a number of hyperelastic compressible and incompressible material descriptions are implemented. The results of thin-walled reinforced hoses and other thin-walled structures will be compared with solutions of the laminat theory. In order to compare the results of multilumic pressure hoses with experimental data a special measuring device and program was created. The influence of different geometrical, structural and material parameter changes will be examined. Different cases of failure are numerically simulated and possibilities of optimization will be shown.

ON FINITE ELEMENT APPROXIMATION OF A NONLINEAR RADIATION PROBLEM

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It is known from physics that each body losses heat energy from its surface by electromagnetic waves. This phenomenon is called *radiation*. The energetical losses are proportional to the fourth power of the surface temperature (the Kirchhoff law). Thus the radiation cannot be neglected when the surface temperature is high (e.g., in computation of temperature distribution in large dry transformers, electrical engines,...). It is represented by the nonlinear boundary condition

$$\alpha(u - u_0) + n^T A \cdot \nabla u + \beta(u^4 - u_0^4) = \tilde{g},$$

where $\alpha \geq 0$ is the coefficient of convective heat transfer, u is the temperature of the body, u_0 is the surrounding temperature, n is the outward unit normal to the surface, A is a symmetric uniformly positive definite matrix of heat conductivities, $\beta = \sigma f_{em}$, σ is the Stefan-Boltzmann constant, $f_{em} > 0$ is the relative emissivity function and $\tilde{g} \geq 0$ is the density of surface heat sources.

Consider the following classical formulation of the radiation problem: Find $u \in C^2(\overline{\Omega})$, $u \geq 0$, such that

$$-\nabla(A \cdot \nabla u) = f \quad \text{in } \Omega,$$

$$u = \bar{u} \quad \text{on } \Gamma_1,$$

$$\alpha u + n^T A \cdot \nabla u + \beta u^4 = g \quad \text{on } \Gamma_2,$$

where $\Omega \subset R^d$, $d = \{2, 3\}$, is a bounded domain with a Lipschitz-continuous boundary $\partial\Omega$, Γ_1 and Γ_2 are non-empty disjoint sets, which are relatively open in $\partial\Omega$, and satisfy $\partial\Omega = \overline{\Gamma_1} \cup \overline{\Gamma_2}$, $f \geq 0$ is the density of body heat sources, $\bar{u} \geq 0$ is the prescribed temperature and

$$g = \tilde{g} + \alpha u_0 + \beta u_0^4.$$

We prove two convergence theorems for piecewise linear finite element solutions for the above radiation problem.

BOUNDARY LAYER RESOLVING FINITE ELEMENT METHOD

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In this work a new finite element method is presented for the solutions of the convection-diffusion equations processing boundary layers. Suitable transformations are first applied to the equations to stretch the boundary layers. Finite element approximation is then considered for the transformed equations which are in general highly degenerate. To approximate such equations efficiently, new finite element spaces which can cope with the degeneracy are investigated. Two possible such finite element spaces are proposed, one of which is non-conforming. Error analysis is presented for the two schemes and numerical tests are reported.

MODELLING OF PLASTIC STRAIN LOCALIZATION IN DYNAMIC LOADING PROCESSES

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The investigation of localized shear band phenomenon, when softening occurs, requires the using of any regularization method which assures the well-posedness of the problem. Each of the proposed methods (e.g. nonlocal theory, second order gradient, Cosserat media or rate dependency) introduce explicitly or implicitly a length scale parameter. To some extent the assumptions made in those methods have their physical explanations, and those methods of regularization can be successfully used for brittle and ductile materials.

In particular, for dynamic processes in ductile materials it seems that the rate dependent formulation (e.g. viscoplasticity) has a good physical background and serves as a regularization method specially when plastic shear band and local softening occur. In this case the relaxation time is used as a regularization parameter.

The problem of mesh sensitivity for regularized FE solutions has been studied by the author for both: critical state line type material (Cam-Clay) and ductile material. The theory of viscoplasticity used in this presentation takes into consideration also the effects of microdamage, thermomechanical coupling and introduces a failure criterion.

The procedure proposed assures the stable integration algorithm. The attention is focused on the well-posedness of the evolution problem and also the convergence, consistency and stability of the discretized numerical problem. For softening materials this discussion is crucial before we start any computations.

The numerical results are obtained in the environment of ABAQUS FE programme and are compared with the available experimental data for a split Hopkinson bar.

* The support of the University Grand DS- /96 is acknowledged. The computations have been performed in Poznan Supercomputing and Networking Center (PCSS) on CRAY-YMP.

USING OF SPECIAL CONSISTENT DISPLACEMENT FIELD APPROXIMATION FOR FINITE-ELEMENT MODELLING OF COMPOSITE STRUCTURES. SOME APPLICATION TO THICK PLATES AND SHELLS

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A special consistency conditions are proposed to define an approximation of displacements through the thickens in the refined displacement-based theories. The consistency conditions are formulated in implicit form and appropriate for creation of applied theory of arbitrary order and any complete set of functions used for displacement-field approximation. The special consistency conditions that were formulated, used as performance criterion of other types refined theories of composite plates and shells. It was establish that theory Donnel-Timoshenko- Mindlin is correct theory, but the approximation of displacements of some wellknown theories are not satiefy to consistency conditions.

The modified finite element approach, based on a set of consistent refined theories of composite plates and shells have been developed and used for numerical analysis of locally loaded fixed composite structures and to define edge stresses in laminates.

A numerical analysis of a group of consistent theories has been conducted in comparison with some variants of applied refined theories. It was found, that correct theories provide simultaneous approximation of all components of the stress-strain state. In the cases, where loads or stresses are fast changed, application of those theories that not satisfied the consistency conditions could lead to significant errors.

An algorithm based on superposition of a number of successive finite element solutions is developed. A problem of combining of finite elements, corresponding to refined theories of different orders is taken into account.

The proposed approach allows to control convergence and precision on each step of solution. Its accuracy is illustrated by series of numerical tests for thick plates

THE *HP*-VERSION WITH THE GEOMETRIC MESH IN 3D-BEM

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The Dirichlet and Neumann screen problems of the Laplacian on open surface pieces (screens) in \mathbb{R}^3 with polygonal boundary can be formulated equivalently as first kind integral equations with weakly singular and hypersingular kernels respectively. Our numerical experiments show exponentially fast convergence of the *hp*-version of the BEM for those integral equations. These results are confirmed by our error analysis which is done in the framework of countably normed spaces [3, 4].

The solutions of the screen problems like solutions of three-dimensional elliptic boundary value problems in polyhedral domains have edge and corner-edge singularities (see [5]), belonging to countably normed spaces, which are also inherited in the solutions of the equivalent first kind boundary integral equations.

In general these singularities diminish the rate of convergence of the standard *h*- or *p*-versions of the boundary element method. Combining the *h*- and the *p*-version in the right way, we obtain here exponentially fast convergence of the BEM. Thus we extend the corresponding results for integral equations on curves to surface pieces.

Recently the exponential convergence of the *hp*-version for the finite element method was proposed for 3D problems in [1] making use of the framework of countably normed spaces (for 2D problems see [2]). Whereas the analysis in [1] requires the use of special meshes our analysis allows to use much simpler meshes due to the tensor product structure of our approximating subspaces of the boundary element *h*-*p* version. Furthermore we deal with screen problems which are not covered by [1].

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MOVING MESH FICTITIOUS DOMAIN METHOD FOR SHAPE OPTIMIZATION

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A novel fictitious domain approach for shape optimization is considered in the case of Neumann boundary value problem for a second order elliptic operator. The main idea is to relax the requirement to have a rectangular mesh during the shape optimization. The topology of mesh is fixed, but the whole mesh is moving. This way it is possible to avoid the non smoothness of cost function, which is a typical problem when fictitious domain methods are used in the shape optimization. The preconditioner is the Laplace operator discretized using a rectangular mesh. Under mild conditions for the mesh deformations it is shown that the condition number of the preconditioned system of linear equations is independent of mesh step size. The minimization of drag of airfoil in 2D full potential flow is considered as a numerical example.

THE APPLICATION OF THE MATHEMATICAL MODEL OF THE TRANSPORT OF CHEMICAL SUBSTANCES DISSOLVED IN THE UNDERGROUND WATER

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A large contamination of the Cenomanian aquifer in the area of the Stráž deposit due to chemical mining of uranium is one of the most important ecological problems in Czech Republic.

This contribution is devoted to the applying of the mathematical model of the transport of chemical substances dissolved in the underground water. Here we want to show some experiments and practical use of the model in the case of remediation of the consequences of the chemical mining of uranium in the North Bohemian region. The use of the model for modelling of pollution leakage from the waste ponds will be shown as well.

For modelling we use the most general mathematical model consisting of porous media fluid flow problem, transport of the chemical substances with diffusion and

dispersion influences and thermodynamical modelling of chemical processes. The brief description of the model will be stated.

MIXED-HYBRID FEM FOR CONVECTION-DIFFUSION TRANSPORT OF CHEMICAL SUBSTANCES DISSOLVED IN THE UNDERGROUND WATER

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A large contamination of the Cenomanian aquifer in the area of the Stráž deposit in Northern Bohemia due to chemical mining of uranium is one of the most important environmental problems in Czech Republic.

This lecture is devoted to mathematical modelling of transport of dissolved chemical substances. The model being used consists of porous media flow and convection-diffusion transport of chemicals with chemical reactions. Several finite element formulations (i.e. primal, mixed-hybrid and mixed) of flow and transport problems are considered due to various requirements of individual modelling tasks. For spatial discretization, trilateral prismatic elements are used to describe the structure of stratified layers.

Results of numerical experiments and practical computations including simulation of remediation schedules in the area of leaching fields and modelling of pollution leakage from waste ponds will be discussed.

THE MODELLING OF DIFFUSION IN CERAMIC MOLDINGS DURING PYROLYSIS

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A general numerical programme was developed to calculate the transient diffusion of degradation product in a ceramic molding during pyrolysis. The differential equation was applicable to a sphere, an infinite plate and an infinite cylinder. The solution includes the concentration dependent diffusion coefficient for diffusion of monomer in its parent polymer which forms the continuous phase in the ceramic in the as-molded state. In the early stages of pyrolysis, before continuous porosity has developed, the model searches for the critical heating rate above which defects are produced. The model was experimentally verified.

ALGORITHMS AND FINITE ELEMENT FORMULATIONS FOR LARGE-STRAIN ELASTOPLASTIC DEFORMATIONS OF SHELLS

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The presentation discusses recent advances in the formulation and numerical analysis of constitutive models for large-strain elastoplastic material response and their implementation into discrete shell-type finite element models. Typical applications are the numerical solution of initial-boundary-value problems in the context of forming processes in thin-walled structures. Key point of the lecture on the side of theoretical modelling in continuum mechanics is the presentation of a new constitutive framework of anisotropic elastoplasticity at large strains based on the notion of a plastic metric, which has been recently proposed by the author. For this material class we point out in detail methodical approaches to implicit integration algorithms of the local evolution equations, which can be recast into the form of general return mapping schemes. In this context, we first propose a new stress-update algorithm for the special case of isotropic elastoplastic response, which can be formulated in the Lagrangian as well as the Eulerian space of principal stretches and stresses for general coordinate charts. Next, we propose return mapping algorithms for the general anisotropic case of the constitutive model mentioned above. Both algorithms are well suited for the implementation in finite element formulations of shell-type continua, which are typically formulated in terms of curvilinear coordinates. In this context, we give an overview about recently proposed finite element formulations for shells based on assumed-strain and enhanced-strain mixed variational methods, which are suitable for the implementation of the general three-dimensional constitutive model discussed above. Key point is the local parametrization of the shell in terms of six independent degrees, including a thickness stretch parameter, which allows the construction of an interface to the material model without shell-specific modifications. We demonstrate the performance of the proposed algorithmic formulation for a spectrum of model problems and benchmarks of general three-dimensional and shell-type elastoplastic continua.

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ERROR ESTIMATES FOR SUBGRIDDED FDTD SCHEMES IN COMPUTATIONAL ELECTROMAGNETISM

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Local meshing or sub-gridding has been advocated by a number of authors as a way of increasing the spatial resolution of the finite difference time domain method (FDTD). The concept is also used in other areas, for example in wave propagation.

In this talk, we start by giving a standard analysis of the spurious reflection that occurs at an interface between two grids for the usual FDTD scheme. This serves as a baseline to compare our analysis of subgridding schemes. We next show how to use supraconvergence techniques to analyze the error in a simple sub-gridding strategy in two dimensions. This strategy is based on constant interpolation (or one sided integration if the method is viewed as a finite volume scheme). Surprisingly the method is found to converge at least at order $3/2$. Experimentally, the rate is second order which is the same as for the standard Yee scheme.

To give a more detailed picture of the error induced by the step change in the grid, we also analyze the spurious reflection that occurs at an interface between two grids of different size for the simple subgridding method and for another subgridding scheme employing linear interpolation. The overall order of convergence of the reflection coefficients is the same for all the methods, but the linear scheme has a lower amplitude spurious transmitted mode compared to the simple subgridding scheme.

We expect our analysis to carry over to the FDTD discretization of the full three dimensional Maxwell system, and an effort to carry out this analysis is under way. The inclusion of time stepping error in the analysis is also necessary.

FINITE ELEMENT METHODS FOR VISCOUS COMPRESSIBLE FLOWS

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Considerable attention has been given in recent years to the application of unstructured mesh methods to the solution of problems involving compressible inviscid high speed flows. As a result, significant achievements have been made in the areas of 3D automatic unstructured tetrahedral mesh generation and solution algorithm performance.

However, the unstructured mesh approach has had very little impact to date in the area of viscous flow modelling. This is due to the fact that the ease with which complex configurations can be meshed is frequently offset by the difficulties associated with the generation of the highly stretched grids, which are efficient for the computation of viscous aerodynamic flows. Attempts have been made to incorporate structured grid concepts by either 'inflating' surface triangulations or utilising hybrid approaches in which structured and unstructured grids are combined. Although some success has been achieved in this way, these approaches are found to often lack geometric flexibility, to require excessive user intervention and to frequently produce low quality grids which are unsuitable for accurate flow computations.

In this paper, we will describe a procedure for generating unstructured tetrahedral grids suitable for high speed flow simulations which addresses some of these recognised difficulties. The approach is based upon the use of conventional algorithms to achieve directional refinement of an existing mesh and allows for the automatic generation of stretched grids, exhibiting tetrahedra in which the largest angle is close to 90 degrees. The proposed method is found to be very effective at generating elements stretched along one direction. This means that the grids produced can therefore result in considerable efficiency gains not only in the calculation of viscous flows but also for inviscid flows, where leading and trailing edges can now be efficiently discretised. The approach requires very little information in addition to that normally provided to an unstructured mesh generator, with the directional refinement being driven by a scalar distance function to a curve or surface.

Several examples will be presented which illustrate the meshes produced by the method when it is applied to aerospace configurations. A solution algorithm, which includes a two-equation turbulence model, will be outlined and experiences gained in the simulations of a number of aerodynamic flows will be described.

ADAPTIVE MULTILEVEL BOUNDARY ELEMENT METHODS IN 3D

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We consider weakly singular and hyper singular integral equations on screens in \mathbb{R}^3 . To obtain approximate solutions we use the h - and p -versions of the Galerkin Boundary Element Method. The Multilevel Additive Schwarz operator with a hierarchical basis yields a preconditioned linear system whose condition number grows only logarithmically with the discretization parameters h or p .

We use the properties of the hierarchical basis to derive an *a posteriori* error estimate for the difference between the exact solution and the additive multilevel solution. For uniform meshes we show reliability and efficiency of our estimate. Based on this estimate we introduce an Adaptive Multilevel Algorithm with easily computable local error indicators and direction control. The theoretical results are illustrated by some numerical examples for h - and p -adaptivity.

FINITE-ELEMENT METHODS FOR ELECTROMAGNETIC FIELD COMPUTATIONS

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Finite-element methods for modeling electromagnetic fields are known to be complicated for at least two different reasons.

First, the finite-element modeling of electromagnetic fields requires a technique for taking into account the discontinuities in components of the field strength (or the flux density) across interfaces where the constitutive coefficients jump. Several methods to solve, or circumvent, this difficulty are known in the literature. We propose a method that offers an optimum in terms of computational efficiency. It basically consists of using an expansion of the field strength (or flux density) in terms of edge (or face) elements along the interfaces where the constitutive coefficients jump and of using nodal elements elsewhere, i.e. in the subdomains where the constitutive coefficients are continuously differentiable with respect to the spatial coordinates. In this way we combine the best properties of both type of element [2].

Secondly, finite-element methods for modeling electromagnetic fields are often haunted by so-called spurious solutions. Spurious solutions are erroneous solutions that may be obtained even when all basic field equations are satisfied accurately. The reason for this is that although the basic equations are satisfied accurately, some of their properties, the compatibility relations [1], may have been lost due to the discretization process. The only way to solve this difficulty is to add the electromagnetic

compatibility relations explicitly to the finite-element formulation of an electromagnetic field problem.

In our talk we will describe the general philosophy underlying our approach and discuss a number of specific aspects of it, stressing the importance of a careful choice of the formulation and the type of expansion to be used. A numerical example will be presented.

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NON-NEWTONIAN FLOW MODELLING FOR THE PROCESSING INDUSTRY

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This paper describes the use of a transient finite element program to solve rheologically complex flows of relevance to the processing industry. Examples may be found in the polymer, oil and food processing sectors, involving applications such as injection moulding, extrusion and mixing. Here we elaborate on the material characterisation and the use of nonlinear viscoelastic models, suitable for shear-dominated and extension-dominated flows.

A Taylor-Galerkin/pressure correction scheme is employed that utilises Petrov-Galerkin streamline upwinding and a time accurate procedure to achieve steady state solutions. This introduces a fractional staged scheme of solution per time step cycle, within which both iterative and direct solvers are invoked. Though the scheme possesses semi-implicit properties, it is element-based, which makes it practical to solve large complex systems of coupled non-linear partial differential equations of mixed parabolic-hyperbolic type. This is typical of the mathematical problems associated with viscoelastic fluids.

A number of practical examples are cited relating to extrusion-coating flows of polymer melts. Here, it is vital to gain insight into the nature of the process to indicate how to optimise its design with respect to processing geometry and effect of rheological material property variation.

FINITE ELEMENT APPROXIMATION OF SHAPE OPTIMISATION PROBLEM FOR NONLINEAR CONTACT SYSTEMS

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The paper deals with the numerical analysis of a shape optimal design problem of large displacement contact problem with the prescribed friction. The equilibrium state of the large displacement contact problem is described by a nonlinear elliptic variational inequality of the second order where the first Piola-Kirchhoff tensor is a coefficient. This problem has at least one global solution, in general nonunique. Conditions of the existence of the local unique solutions to this problem, based on its linearization and their regularity are studied in literature. Numerical algorithms for solving large displacement contact problems are based on the existence of local unique solutions.

Shape optimization problem for large displacement contact problem consists in finding, in a contact region, such shape of the boundary occupied by the body in its reference configuration that the normal contact stress is minimized. It is assumed that the volume of the body is constant.

In this paper we formulate the nonlinear contact problem employing the mixed variational approach where the deformation and the tangent contact traction are independent variables. The cost functional approximating the normal contact stress will be introduced and shape optimization problem will be formulated. Using the material derivative approach as well as the results of differentiability of solutions to the variational inequality we calculate the directional derivative of the cost functional and we formulate a necessary optimality condition. The calculated directional derivative will be used in numerical algorithm in descent direction finding procedure. The optimization problem will be approximated by the finite element method. The convergence of the approximation is proved. Finally, the discretized optimization problem is numerically solved by the algorithm based on the Augmented Lagrangian Technique combined with the projected gradient type algorithm. Numerical examples are provided. For the sake of simplicity we shall deal in this paper with static model only, however our approach can be extended to quasistatic contact models as well.

A SCHWARZ ADDITIVE METHOD WITH HIGH ORDER INTERFACE CONDITIONS AND NONOVERLAPPING SUBDOMAINS

F. Nataf

ADDRESS NOT SUPPLIED

The convergence of a Schwarz additive method is proved for a nonoverlapping decomposition into rectangles with interface conditions of order two in the tangential direction.

The whole paper is available as a compressed Postscript file by internet procedure FTP anonymous on host `barbes.polytechnique.fr` (129.104.4.100) in the directory `pub/RI/1996` under the name

`nataf_339.janv.ps.gz`

or by Xmosaic or any other www client via the CMAP www server

`http://blanche.polytechnique.fr/`

FINITE ELEMENT PREDICTION OF FLOW IN A PERISTALTIC BLOOD PUMP

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The paper presents an application of Computational Fluid Dynamics to the fluid flow in a novel peristaltic blood pump. The work is aimed at obtaining a better understanding of the fluid behaviour, pressure and shear stress distributions in the fluid.

A major difficulty to overcome in the design of blood pumping systems is to avoid cellular damage. It is also required that the pump does not contaminate the blood. A common way of designing pumps to meet these requirements is to use rotary peristaltic pumps. In such a pump the fluid is pumped by the action of rollers on the outside wall of a flexible tube that these pumps still cause damage as a consequence of high contact forces and localized viscous shear stresses.

A novel peristaltic pump has been developed at Brunel Institute for Bioengineering. The motivation for the development of this new pump is to reduce blood damage. The prototype model is made of a single silicon tube surrounded by three independent pumping chambers. The the pressure cycles in the three chambers are synchronised, the fluid is pumped peristaltically in one direction. Compared with others, this pump uses a linear peristaltic action to move the fluid.

The present work is as part of a wider investigation to optimise the design of the pump. It uses a finite element method of solving the governing differential equations. The computer code used for this purpose is FIDAP.

The model comprises a tube filled with fluid surrounded by three chambers. The fluid flow is treated as unsteady, laminar, Newtonian and axisymmetric. The boundaries of these channels move independently with a prescribed sinusoidal function.

The results are presented for the velocity field, pressure, shear stress and rate of flow as a function of time. Animations of the velocity field are produced which clearly show the pumping characteristics of the model.

OPTIMAL CONTROL WITH A VARIABLE RESOLUTION FINITE ELEMENT SHALLOW WATER EQUATIONS MODEL

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The adjoint model of a finite-element shallow-water equations model was obtained with a view to calculate the gradient of a cost functional in the framework of using this model to carry out variational data assimilation (VDA) experiments using optimal control of partial differential equations. The finite-element model employs a triangular finite-element Galerkin scheme (Navon 1983) and serves as an prototype of 2-D shallow-water equations models for tackling computational problems related to optimal control of distributed parameters with finite-element numerical weather prediction models.

The derivation of the adjoint of this finite-element model involves overcoming specific computational problems related to obtaining the adjoint of iterative procedures for solving systems of non-symmetric linear equations arising from the finite-element discretization and dealing with irregularly ordered discrete variables at each time-step. Robust large scale numerical optimization algorithms are also required.

Using the initial conditions as control variables, a cost function was minimized consisting of the weighted sum of differences between model solution and model generated observations. An additional set of experiments was carried out evaluating the impact of carrying out VDA involving variable mesh resolution in the finite-element model over the entire assimilation period. Several conclusions are drawn related to the efficiency of VDA with variable horizontal mesh resolution finite element discretization and the transfer of information between coarse and fine meshes.

NUMERICAL SOLUTIONS OF A COUPLED TWO-PHASE STEFAN-CONTACT PROBLEMS WITH FRICTION IN THERMOELASTICITY BY A VARIATIONAL INEQUALITIES

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In this paper we shall investigate the model of a collision zone, which render to study also recrystallization and melting of rocks in collision zones and in their close and longer neighbourhoods. The own problem investigated represents a simulation of geodynamic processes in collision zones, based on the plate tectonics and contact problems with or without friction in linear thermo-elasticity as well as two-phase Stefan problem. The weak formulation of the contact part of problem thus results in an elliptic variational inequality, while a semi-implicit discretization in time of the weak formulation of the Stefan problem using the enthalpy approximation results in an elliptic boundary value problem and therefore leads to an elliptic variational inequality. Numerically then the problem yields the finite element approximation of a coupled contact-Stefan problem in linear thermoelasticity. The linear finite elements will be used and the convergence of the FEM approximation of the solution to the weak solution of the coupled contact-two-phase Stefan problem will be proved.

HOMOGENIZATION AND MULTIGRID

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One difficulty for computation of flows in porous media is their extremely complex structure. Therefore, in many cases homogenized equations will have to be used, sometimes this procedure will even have to be done on several scales.

We consider multigrid methods for which such a change of law is important, i.e. the fine grid equations are totally different from the coarse grid ones. First, we show convergence of a multigrid method that uses coarse grid equations motivated by analytic homogenization. Second, we demonstrate the efficiency of this method in comparison to algebraic multigrid methods.

SOLUTION OF SINGULAR PROBLEMS USING H - P CLOUDS

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The behaviour of the $h - p$ cloud method [2, 1] for the analysis of boundary-value problems with singularities is analyzed. Two approaches to model singularities associated with re-entrant corners are investigated. In the first technique, the meshless character and the ability of the $h - p$ cloud method to implement h , p and $h - p$ adaptivity without traditional mesh concepts are explored. An a posteriori error estimate is used to derive the adaptive process. The second approach explores the ability of the $h - p$ cloud method to include in its approximating spaces specially tailored functions to model singularities. This technique is used to analyze an edge-cracked panel.

A new approach for the extraction of the amplitude of the singular terms associated with corner singularities is also presented. The extraction procedure requires a straightforward implementation and numerical experiments show that the extracted quantities converge at the same rate as the strain energy of the problem and, therefore, at twice the rate of the error in the energy norm.

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SOME ADVANCED COMPUTATIONAL STRATEGIES FOR THE MODELLING OF FORMING PROCESSES

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Introduction

This paper discusses some issues in the computational treatment of non-linear problems which have arisen out of the necessity to solve various classes of industrial forming problems. Although the applications considered are taken from a range of commercial sectors, the principal numerical challenges are largely common. The main issues relate to the implementation of advanced constitutive models under conditions of finite strain elastic and inelastic deformations, element methodology for incompressible behaviour, mesh adaptivity strategies and equation solution procedures for large scale problems.

Constitutive Modelling

A basic requirement of the computational modelling of non-linear material behaviour under finite strain conditions is the consistent linearisation of the discretised equations. The development of consistent tangent operators becomes progressively more difficult with increasing complexity of the constitutive models employed. For example, simulation requirements for industrial operations involving powder compaction and soft solids processing has lead to the introduction of pressure dependent constitutive laws of the Gurson and crushable foam types. Problems associated with the efficient computational implementation of such models within a finite strain setting are discussed.

A main development concerned with modelling frictional contact phenomena is the description of a model particularly suited to coated sheet materials. A model is described which is based on the plasticity theory of friction in which a hardening variable is introduced to represent the dependence of friction on the degree of relative sliding between the tool and workpiece. Attention will also be given to the development of a computational procedure for predicting tool wear.

Adaptivity with Evolving Geometries

A general feature encountered in the finite element simulation of forming operations, such as forging or deep drawing, is that the optimal mesh configuration changes continually throughout the deformation process. Therefore, the introduction of adaptive mesh refinement processes is crucial for the solution of large scale industrial forming problems, which necessitates (i) a remeshing criterion, (ii) specification of an appropriate error estimation criterion, (iii) development of a strategy for adapting the mesh based on the error distribution and (iv) automatic mesh generation tools.

For forming problems, in which the geometric changes are usually large, the decision to update the finite element mesh is invariably based on element distortion parameters and the role of error estimation is then to decide the element size distri-

bution in the new mesh. In view of its fundamental importance to inelastic problems of evolution through the second law of thermodynamics, an error estimation strategy based on the plastic dissipational functional and the rate of plastic work is introduced. For problems involving non-linear behaviour, and plastic deformation in particular, issues related to the transfer of variables from the old mesh to the new mesh are crucially important for preserving the robustness and convergence properties of the finite element solution. Problems in this area become especially acute when deformations are large, resulting in evolving geometries as is the case in forming simulations. When mapping from the old to new mesh, (i) Consistency with the constitutive equations, (ii) The requirements of equilibrium, (iii) Compatibility of the state transfer with the displacement field on the new mesh, and (iv) Compatibility with evolving boundary and loading conditions must be satisfied. A transfer strategy for large strain elasto-plastic problems is described in which the current displacement field and the plastic part of the deformation gradient corresponding to the previous converged solution is employed for state transfer.

Explicit Solution Strategies

The excessive computational times associated with implicit quasi-static solutions of forming problems has lead to the extensive use of explicit time integration procedures. Typically, for large scale 3D problems solution by the explicit method can be accomplished at least one order of magnitude faster than the corresponding implicit analysis. However, inertia effects have no significant influence in most forming operations and efficient explicit solution of these essentially quasi-static problems depends on choice of artificial values for parameters such as the material mass and process speed. The paper discusses issues related to the efficiency and accuracy of explicit solution procedures for forming problems and also illustrates the role of mesh adaption strategies.

Element Methodology

A fundamental requirement for bulk forming simulations is the use of appropriate elements which can model the incompressible nature of the plastic flow without exhibiting locking behaviour. The tendency of the solution to lock, that is provide over stiff solutions with poor stress representation, becomes more predominant when large deformations are involved, as is the case in all forming operations. In addition to producing unacceptable stress fields within the workpiece, this also leads to a poor representation of surface tractions and hence to incorrect prediction of contact/friction conditions between the tools and workpiece. The paper discusses some of the more popular strategies employed to overcome these difficulties. One effective solution to this problem is offered by the F-bar element in which a multiplicative split of the deformation gradient is employed to enforce the incompressibility constraint. The element is free from hourglassing defects, exhibits a relatively large bowl of convergence and is especially suitable for adaptivity applications.

Equation Solution and Parallel Processing

The ever increasing need to solve large scale industrial problems by an implicit approach demands that advances be made in equation solution strategies. As equation systems extend beyond a certain size (of the order of 20,000 dof), direct solvers become increasingly inefficient and iterative solvers offer the most natural approach

to solution. Currently, the most promising candidates are Conjugate Gradient (CG) or multi-grid techniques. CG methods are commonly employed, with various preconditioning strategies utilised to improve the conditioning of the equation system (e.g. Jacobi, Incomplete Cholesky, etc.). Considerable promise is also offered by multi-grid methods; in which the problem is first solved on a coarse mesh to precondition the equation system for subsequent solution by CG on a finer mesh. Issues related to the solution of large scale problems by iterative solvers are discussed.

The rapid emergence of parallel processing hardware, even at the multi-processor workstation level, necessitates consideration of solution methods for forming problems by concurrent computational methods. In this respect domain decomposition techniques offer efficient parallel implementation and can be utilised on both shared and distributed memory computers. Furthermore, they are applicable to both implicit and explicit solution algorithms. Issues which require detailed consideration are load balancing, memory allocation and data communication, with a need to provide generic solution strategies in addition to solutions for specific architectures. Implementation issues are discussed, including the treatment of evolving contact conditions.

SHAPE OPTIMIZATION FOR A MIXED BOUNDARY VALUE PROBLEM AND A STOKES PROBLEM

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The problem of estimating the shape of the boundary based on interior measurements of the solution of an elliptic boundary value problem and a Stokes problem is considered. In order to overcome the numerical complexity of repeatedly solving the PDE on a sequence of curvilinear domains of varying shapes an embedding domain method for mixed boundary value problems and a Stokes problem is derived. The derivative of the cost with respect to the shape is characterized in terms of the Lagrange multipliers for the primal and the adjoint problems. Numerical results illustrating the efficiency of the method which is related to a mixed finite element method are presented.

NUMERICAL RESULTS USING A COMBINED BOUNDARY ELEMENT AND FOURIER METHOD

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The numerical solution of a boundary integral equation for time harmonic screen problems is discussed. A singularity function approach, based on explicit inverses for the Laplace equation, is used. Convergence orders for Galerkin schemes and numerical results are presented. The difficulties concerning numerical implementation and some limitations of the method are discussed.

A THREE-DIMENSIONAL BOUNDARY ELEMENT MODEL FOR A SOIL-STRUCTURE INTERACTION PROBLEM

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The aim of this study is to determine the influence of the dynamical properties of track and the underlying soil on generation of ground vibration due to surface railways. The rail is modelled as a point force, excited, infinite Euler-Bernoulli beam. The supports are modelled as lumped mass-spring-damping systems, and have a dynamic stiffness. When *soil-loading* is neglected the response to a point force may be evaluated explicitly by contour integration. In particular a *dispersion relation* between the wavenumber of the beam and the *propagation constants* is determined. From this relation so called pass-band and stop-band regions may be evaluated for the infinite beam. The vertical response of the beam at the load point is calculated for a frequency range up to 1000 Hz. Certain well known characteristics of the response are presented.

When *soil-loading* is included the boundary element method for the soil region generates a dynamic stiffness matrix for the periodic supports. Numerical methods are used to calculate the vertical response for the beam and the subsequent vibration propagating through the ground.

MODELLING THE CONFIGURATION OF ELECTRICAL MACHINES FOR 3D-FEM COMPUTATIONS

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Over the past several years the Finite Element Method (FEM), especially in the three dimensional domains, has become an established numerical tool for calculations of magnetic field distribution, and both electromagnetical and electromechanical characteristics of electrical machines. The numerical calculation of the magnetic vector potential and its components is based on the Poisson's equation applied in the 3D domain of the electrical machine which is going to be analysed.

In this paper, modelling of the configuration required for three dimensional field analysis in two types of permanent magnet electrical machines will be presented. The first one is electronically operated synchronous machine (PMSM), having samarium cobalt magnets mounted on the outer surface of the rotor. The second one is DC commutator motor (PMCM), having segmental ferrite magnets mounted on the inner stator frame surface. By an appropriate both geometrical and mathematical modelling of the machine configuration in the whole considered domain, the three dimensional magnetic field solution, by using Finite Element Method will be performed. For the proper determination of characteristics and an accurate analysis of

the phenomena as well as the performance of the permanent magnet electrical machines under various operating and load conditions, it is necessary to calculate the magnetic field distribution as exact as possible. The accuracy of computation of the 3D magnetic field distribution depends on the proper modelling of the electrical machine configuration.

Because of the appropriate geometrical and mathematical modelling of the permanent magnet electrical machines their configuration in three dimensional domain will be divided into several layers along axial axis of the machines, as follows: the active length of the machine (first layer), the winding overhangs (two layers) and upper surrounding area (one to two layers). For the purposes of three dimensional field modelling, the corresponding mathematical model of permanent magnet excitation, suitable to finite element method calculations, taking into account the magnet anisotropy, will be derived. At the same time, the different magnetic reluctivities along the co-ordinate axes, due to lamination of magnetic core, are taken into consideration. As the most suitable shape for the finite element is chosen to be the triangular prism, which enables to consider the rotor or stator skewed slots very simply. Calculations are carried out for various load currents and for different rotor angular positions to the selected referential axis. The mesh of finite elements is particularly adjusted to convenient modelling of the movement of rotor, as well as the winding end-regions outside of the motor active length. After the nonlinear iterative calculations of the magnetic vector potential in the whole investigated 3D-domain will be accomplished, it is possible to get the magnetic field distribution in different axial cross-sections of the analyzed motors. In the full paper there will be presented flux plots for the electrical machines under consideration.

For complex analysis of the behaviour of the electrical machines with stator or rotor mounted permanent magnets, it is necessary to compute both electromagnetical and electromechanical characteristics. Numerical calculation of fluxes is carried out on the basis of the field theory by using numerical integration of the magnetic vector potential calculated by the 3D-FEM. Magnetic flux density will be calculated numerically, too. Electromagnetical torque is one of the most significant quantity for the motor performance and it will be calculated by using the energy concept. The static electromagnetic torque is effected by the magnetic field energy variation in the air-gap at the movement of rotor, for constant armature current. The available database with values of magnetic vector potential obtained as an exit of the numerical 3D field calculation, is quite correspondent with the numerical procedure for calculation of the static electromagnetic torque in electrical motors. For the quasi static model of the both considered motors, the magnetic coenergy and the static electromagnetic torque will be calculated numerically. In the paper there will be presented calculated characteristics for PMSM and PMCM, respectively.

The proposed 3D field modelling applied to permanent magnet motors gives an opportunity for complex calculation of characteristics and an analysis of the motor performance. In the paper will be presented a detailed modelling, including the likenesses and differences of both types permanent magnet motors. The numerically calculated characteristics are compared with the experimentally obtained ones and they show a very good agreement, what proves the methodology as accurate. Hence, the proposed procedure could be used for the prediction of electrical machine characteristics.

LARGE-SCALE MODELS AND CONDENSATION TECHNIQUE OF JOINTS IN TURBOMACHINE IMPELLERS USING SYMMETRY AND MODEL PECULIARITIES

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Turbine or compressor bladed disks consist of different structural members - blades, disk, shrouds. To accurately calculate modal and forced response characteristics it is important to describe adequately interaction between the members. Intricate shapes of blade-disk and blade-shroud joints design, high degree of detail of interaction conditions on contact surfaces and large gradients of stresses cause necessity of large-scale finite element models. To allow use such models in vibration analysis of assemblies of blades, disk and shrouds it is necessary to develop special technique for decrease size of the matrices.

Finite element models of joints are developed and a condensation technique is proposed that is based on accounting of rotationally symmetric properties of bladed disks and model peculiarities of joined components of a bladed disk.

A shroud-blade joint consists of a shroud per one blade and adjoined small part of the blade. A shroud is considered as an intricate shape plate or as a three dimensional solid depending on its design. Adjoined part of blade is considered as a shell or as a three dimensional solid. It is possible to take into account different interaction conditions of neighbouring shroud shelves on whole or any part of contact surfaces. They are: slip in any specified directions, full contact, absence of contact and others.

A shroud-disk joint consist a blade root, a small part of a disk adjoined one blade and the small part of a blade which is near the root. All the members is considered as a three dimensional solid. Any design of blade root and any interaction conditions of neighbouring blades and root with disk may be considered.

The technique takes into account axial symmetry of disk as well as rotationally periodic symmetry of blading and a whole bladed disk. Size of matrices may be decreased from values estimated by thousands down to a few. Effective handling of large matrices during multi-stage condensation process is developed. The technique supply accounting the fact that the joints are parts of blades -disk shrouds assembly. Interaction of joints with other parts of oscillated assembly is simulated without simplified assumptions. Cases of twisted rod and shell models of blades for this assembly are examined.

Software that uses this technique has been developed. Numerical investigations have been carried out and comparison of results calculated by proposed technique, and results calculated by preceding techniques.

The proposed approach may be effectively used for other rotationally symmetric mechanical systems constructed from members described by different models.

DOMAIN OPTIMIZATION PROBLEMS FOR CONTROL OF THIN ELASTIC PLATES

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A class of shape optimization problems associated to optimal location of distributed controls for thin elastic plates is considered. The existence of solutions for optimization problems is established using a regularization technique. The first order optimality conditions are obtained by an application of the material derivative method. A relaxation method is proposed and the resulting parametric optimization problems are analysed.

ELECTROMAGNETIC SCATTERING FROM AN ORTHOTROPIC MEDIUM

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Consider electromagnetic scattering from an inhomogeneous anisotropic medium. For the case of an orthotropic medium we derive the Lippmann-Schwinger equation, which is equivalent to a system of strongly singular integral equations. Uniqueness and existence of a solution is shown and we examine the regularity of the solution by means of integral equations. We prove the infinite Fréchet differentiability of the scattered field in its dependence on the refractive index of the anisotropic medium and we derive a characterization of the Fréchet derivatives as a solution of an anisotropic scattering problem.

THE LOW REYNOLDS NUMBER INTERACTION BETWEEN A SOLID PARTICLE AND A VISCOUS DROP

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The low Reynolds number motion and deformation of a neutrally buoyant drop (immersed in a different viscous fluid) due to its interaction with a translating solid particle (immersed in the same fluid) is studied.

Rallison and Acrivos [3] developed a numerical solution for the low Reynolds number deformation of a viscous drop suspended in a second fluid that is caused to shear, using the Green's integral representation formulae for the fluids inside and outside the drop. By requiring that the flow fields satisfy the matching conditions at the drop interface, they found a second kind Fredholm integral equation for the unknown surface velocity. Power [1] proved, analytically, that Rallison and Acrivos' integral equation possesses a unique continuous solution when $0 < \lambda < \infty$, with λ the viscous ratio, i.e. all possible cases except when the object is a solid particle ($\lambda = \infty$) or a gas bubble ($\lambda = 0$).

In the case of a solid particle, $\lambda = \infty$, Youngren and Acrivos [4] used the integral representation formulae for the exterior Stokes flow around the particle, to obtain a first kind Fredholm integral equation for the unknown surface traction. As is known, Fredholm integral equations of the first kind generally give rise to unstable numerical schemes based upon discretization of the surface integrals involved, the instability manifesting itself in the ill-conditioning of the matrix approximation of the kernel. Nonetheless, it is possible to apply the discretization method if only low-order accuracy is desired. On the other hand, solving an equation of the second kind is a well-posed problem.

Power and Miranda [2] explained how integral equations of the second kind can be obtained for general three-dimensional Stokes flows around a single particle by completing the deficient range of the double layer operator (*Completed Double Layer Boundary Integral Equation Method*).

This work presents a constructive way of finding the hydrodynamic interaction between a solid particle and a viscous drop. This is achieved by means of a system of second kind Fredholm integral equations. The approach presented here is an extension of Power and Miranda's *Completed Double Layer Boundary Integral Equation Method*. It also shows that the resulting system of integral equations possesses a unique continuous solution, and thus the proposed form of solution is assured to provide the unique regular solution of the present interaction problem.

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EXACT NON-LINEAR FINITE ELEMENTS FOR THE ANALYSIS OF THIN PLATES AND SHELLS

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In the last three decades many finite element solutions for the non-linear problems in thin elastic plates and shells have been developed. A usual practice in most of these solutions is the separation of rigid body movements from the local deformations and the use of linear elements to model the structure at local level. The effect of large displacements is then introduced through the transformation from local to global coordinates. The main advantage of such techniques is the extension of their application into a whole range of geometrically non-linear problems including finite rotations. However, in order these techniques to yield meaningful results the element size should be small. Furthermore, these formulations do not have the theoretical background to recover exact geometrically non-linear solutions for a finite mesh.

The present paper contends with a rather different approach and examines a new generation of flat triangular finite elements which are inherently non-linear and are exact according to the theory of von Kármán for thin plates. They are suitable for the solution of problems where the in-plane rotations are small and the out of plane rotations are moderate. It is recalled that this is satisfactory for most engineering purposes because most shells would become completely unserviceable if really large rotations were permitted. The theoretical basis for the development of this type of finite elements has been set recently by Morley who derived a six noded flat triangular element with constant moments. This element because of its simplicity and integrity is ideal for the purpose of fundamental research.

A more practically useful element is the three noded triangle with the desirable three displacement and three rotation connectors at each corner. A such geometrically non-linear triangle is described here. The element is derived by the means of the modified generalised Hu-Washizu variational principle and the Total Lagrangian formulation. Inside the element the in-plane and the out of plane displacements are taken to be quadratic and cubic polynomials respectively. Along the element boundary the in-plane displacement is assumed to vary linearly, the out of plane displacement to vary cubically and the normal rotation to vary linearly. The element matrices are derived through explicit calculations and no use of various artificial means such as numerical integration is made.

Numerical examples presented here demonstrate very good performance. Exact non-linear finite elements are expected to be very useful to both the engineering and mathematical community. They are going to facilitate the error estimation which at present is mainly restricted to linear plate formulations.

NUMERICAL MODELLING OF MULTIPHASE IMMISCIBLE FLOW IN DEFORMING POROUS MATERIAL AND ITS APPLICATION TO SUBSURFACE CONTAMINATION

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A numerical model is developed that describes multiphase flow through soil involving three immiscible fluids: namely air, water and a nonaqueous phase liquid (NAPL) in deforming porous media. The governing equations in terms of soil displacements and fluid pressures are coupled non-linear partial differential equations and are solved by the finite element method. Two-dimensional simulations are presented for a hypothetical field case involving introduction of NAPL near the soil surface due to leakage from an underground storage tank. Subsequent transport of NAPL in the variably saturated vadose and groundwater zones is analyzed.

ERROR ESTIMATES AND EXTRAPOLATION FOR THE NUMERICAL SOLUTION OF MELLIN CONVOLUTION EQUATIONS

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We consider a quadrature method for the numerical solution of a second kind integral equation over the interval, where the integral operator is a compact perturbation of a Mellin convolution operator:

$$\tilde{x}(\tilde{t}) + \int_0^1 \tilde{k}(\tilde{t}, \tilde{s}) \tilde{x}(\tilde{s}) d\tilde{s} = \tilde{y}(\tilde{t}), \quad 0 < \tilde{t} < 1, \quad (1)$$

$$\tilde{k}(\tilde{t}, \tilde{s}) = \tilde{k}_M \left(\frac{\tilde{t}}{\tilde{s}} \right) \frac{1}{\tilde{s}} + \tilde{k}_S(\tilde{t}, \tilde{s}), \quad 0 < \tilde{t}, \tilde{s} < 1.$$

Our quadrature method relies upon singularity subtraction and transformation technique. Stability and convergence order of the approximate solution are well known. Since the solution \tilde{x} of (1) has an asymptotic behaviour $\tilde{x}(\tilde{t}) \sim C + \tilde{t}^\gamma$, $\tilde{t} \rightarrow 0$ with C a constant and $\gamma > 0$, the numerical solution \tilde{x}_h depending on the mesh size h

will also have a special asymptotic behaviour. We shall derive the first term in the asymptotics of the numerical error:

$$\tilde{e}_h(\tilde{t}) = \tilde{x}(\tilde{t}) - \tilde{x}_h(\tilde{t}) = h^\gamma \tilde{f}(\tilde{t}/h) + O(h^n), \quad 0 < \tilde{t} < 1,$$

where $\gamma < \gamma_1$ and $|\tilde{f}(\tau)| = O(\tau^{-\beta})$ for $\tau \rightarrow \infty$ with $\beta > 0$. This formula shows that, in the interior of the interval, the approximate solution converges with higher order than over the whole interval. Moreover, we can derive higher orders of convergence for the numerical derivation of smooth functionals to the exact solution. Finally, the asymptotics allows us to define a new approximate solution extrapolated from the dilated solutions of the quadrature method over meshes with different mesh sizes:

$$\tilde{x}_h^e(\tilde{t}) := \tilde{x}_{2h}(\tilde{t}) + \sum_{l=0}^{L-1} 2^{-l\gamma} \{ \tilde{x}_h(2^l \tilde{t}) - \tilde{x}_{2h}(2^l \tilde{t}) \}.$$

This extrapolated solution differs from the usual Richardson extrapolation and is designed to improve the low convergence order caused by the non-smoothness of the exact solution even when the transformation technique corresponds to slightly graded meshes. We discuss the application to the double layer integral equation over the boundary of polygonal domains and report numerical results.

GLOBAL-LOCAL COMPUTATIONAL PROCEDURES FOR THE MODELLING OF COMPOSITE STRUCTURES

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To accurately capture the localized 3-D stress fields in practical laminated composite structures, it is usually necessary to resort to a simultaneous multiple model approach in which different subregions of the problem domain are modeled using appropriate kinematic structural theories. The objective of a simultaneous multiple model analysis is to match the most appropriate structural theory with each subregion based on the physical characteristics, applied loading, expected behavior, and level of solution accuracy desired within each subregion. Thus solution economy is maximized without sacrificing solution accuracy. While such simultaneous multiple model methods are simple in concept, the actual implementation of such techniques is complicated and cumbersome due mainly to the need for maintaining displacement continuity across subregion boundaries that separate incompatible subdomains.

To overcome the difficulties encountered in the conventional global-local analysis of practical composite laminates, a hierarchical finite element model is developed by the author and his colleagues [1-3]. The displacement field hierarchy included in the model contains both conventional equivalent single-layer and full layerwise expansions. The hierarchical nature of the model permits the computational domain to be divided into different subregions that are incompatible with respect to mathematical model type and level of finite element mesh discretization. The hierarchical model

is a convenient vehicle for the analysis of composite laminates using simultaneous multiple models, and completely overcomes the difficulties associated with enforcing displacement continuity along boundaries separating incompatible subregions. In addition, the hierarchical model provides a convenient means to add progressively higher-order effects to existing models as deemed necessary by previous solutions.

An overview of the theories and the recent research of the author on the global-local computational approach based on the variable kinematic modeling of laminated composite structures is presented. A review of the computational models based on equivalent single-layer assumptions and layerwise expansions is discussed, and the variable kinematic finite element model concept developed by the author is described, and sample applications of the computational procedure are presented.

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COMPARISON OF VARIOUS NUMERICAL METHODS IN THE COOLING OF STEEL

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An industrial Finite Element(FE) package has been developed to allow transient temperature calculations within steel sections, taking account of the non-linearities caused by the highly temperature dependent thermal properties and boundary conditions, and allowing the use of a wide variety of time integration schemes so as to optimise computational efficiency. The simulated cooling of hot-rolled steel sections can take considerable amounts of computer time, so the use of efficient time integration schemes is highly desirable. The performance of special extended-stability explicit Runge-Kutta(RK) formulae has been compared with that of more conventional implicit and explicit methods.

Model simulations of various industrial steel-cooling systems have revealed that the solution is characterised by an initial fast transient phase, in which time step

length is limited by accuracy considerations, followed by a stiff phase, in which step-size is governed by numerical stability. The type of cooling system in use determines the relative duration of these two solution phases, and hence the most appropriate integration scheme. The attraction of integrators with adaptive step-size control is clear. Embedded second and third order RK formulae, developed from families of shifted Chebyshev polynomials with optimised real absolute stability, have therefore been tested as a possibly more efficient alternative to standard integration routines. The economical local error estimates provided by these formulae at each step permit the optimisation of step size during both transient and stiff solution phases, using appropriate adaptive procedures.

Preliminary numerical experiments have shown that the special embedded RK formulae are considerably more efficient than the other explicit methods (forward Euler and "classical" RK methods), and that their performance compares well with standard implicit methods, particularly for problems which exhibit significant transient solution behaviour.

The result of various numerical investigations will be given, covering a range of industrial cooling applications. In such cases reduction in computer run time by a factor of more than five have been achieved.

A SPACE DECOMPOSITION METHOD FOR PARABOLIC PROBLEMS

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In this work, we shall consider a space-decomposition technique for an abstract parabolic equation, including the non-symmetrical case. A convergence proof is presented, and it is shown that if the Euler or the Crank-Nicolson scheme is used for the parabolic problem, only $O(|\log(dt)|)$ steps of iteration is needed at each time level, where dt is the time step size. Applications to overlapping domain-decomposition and to a two-level method are given for a convection-diffusion equation using finite element. Analysis shows that only a one-element-overlap is needed. Numerical test-results are presented.

SHAPE OPTIMIZATION OF ELASTO-PLASTIC BODIES

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The paper deals with the sensitivity analysis and shape optimization of bodies in which the distribution of plastic strains is nonzero in a neighbourhood of the optimal design. The problem belongs to the class of parametric optimization of systems governed by quasi-variational inequalities. A classical regularization technique consists in converting the variational inequality into an equation by means of a smooth penalty. In this way a standard optimal control problem is obtained. However, the smooth penalization leads to a low accuracy or to ill-conditioned problems. The approach applied in this paper uses some tools of nonsmooth analysis to handle the quasi-variational inequality as a nondifferentiable controlled system.

The elasto-plastic behaviour of the material is assumed to be governed by the Huber-von Mises yield function with strain isotropic hardening. In accordance with the incremental theory, the considered mathematical model is presented by the time sequence of the metric projections on the convex sets which are formed by the equilibrium conditions and the yield conditions. The formulation in strain space has been proposed by Hlaváček, Rosenberg, Beagles and Whiteman (1992) and modified by Kuczma and Whiteman (1993). The first formulation uses the hardening function α to determine both the yielding condition and the plastic strain increment. In the second approach the plastic multiplier λ is employed instead of α . As α and λ are related by $\dot{\lambda} = H'^{-1}\dot{\alpha}$, where H' is the tangent modulus, the first formulation via hardening function is not convenient to describe perfect plasticity $H' \rightarrow 0$ as a special case.

The state problem approximated by finite elements in space and finite differences in time can be converted into the set of nonsmooth equations by means of the *implicit complementarity problem*; for a given design parameter $u_0 \in U_{ad}$ find the set $\{y_0^{(i)}\}_{i=1}^t$, so that

$$y_0^{(1)} = S^{(1)}(u_0), \quad y_0^{(i)} = S^{(i)}(u_0, y_0^{(i-1)}(u_0)) \quad \text{for } i = 2, \dots, t.$$

$S^{(i)}$ stands for "system map" corresponding to the solution of the nonsmooth equation at the time level i . The sensitivity analysis of the above time-dependent problem is based on directionally differentiable implicit functions. The subgradient of an objective functional can be obtained using adjoint-equation technique developed for the augmented elasto-plastic model which involves both hardening function α and plastic multiplier λ to include the perfect plasticity. The bundle trust method is tested to cope with the numerical solution of the optimization problem.

2D FEM FOR NUCLEAR MAGNETIC RESONANCE MAGNET DESIGN WITH NEW S-MATRIX PACKED APPROACH

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The results of magnetic field intensity and its spatial inhomogeneity calculations in the cross section of electromagnet by modified finite element method are presented and discussed. The standard triangular elements [2, 1] with linear field approximation are used. Sizes of elements, values of permeability in these elements, magnitudes of current density in coils, magnet pole pieces and coils profiles, the boundary Dirichlet conditions are defined by user of our program MAG-2. The method of packing of the S-matrix (the packed S-matrix takes up only 5% of memory as compared with the initial memory capacity) is the quite novel in this approach. This algorithm is the reason for the considerable increase in the number of elements and reduction in the calculation errors (e.g. if the random access memory of an IBM AT 486DX2 is 640 Kb we can use about 3000 elements for 1/4 of the magnet full cross section). The calculations have been carried out for Nuclear Magnetic Resonance (NMR) magnets with the ratio D/L of the magnet pole piece diameter (D) and the width between pole pieces (L) 2-4. The relative error in the calculation was less than 0.005%. The difference between the calculated and measured data was less than 0.01%. It has been shown that the parameters of magnet: decrease of the weight, materials saving and increase of the spatial field homogeneity may be improved by means air cavities in the magnet pole pieces.

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A PANEL CLUSTERING BOUNDARY ELEMENT METHOD FOR THE IMPEDANCE VALUE PROBLEM FOR THE HELMHOLTZ EQUATION IN A HALF-PLANE

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A piecewise constant semi-describe collocation method is used to solve the impedance boundary value problem of the Helmholtz equation numerically. The boundary integral equation method is used, and the resulting integral equation over the real line is truncated to produce a linear system with a finite number of equations. Error analysis results depending on the parameter of discretization and on the truncation width are presented.

In the second part of the talk we present a lumping scheme to reduce the number of interdependencies in the unknowns of the linear system. Here we make use of the knowledge of the oscillatory behaviour of the kernel of the integral equation. The resulting matrix is sparse and in the cases shown the time needed to solve the linear system is reduced by a factor of 20. The accuracy of the fast solution method is investigated by comparing results with those of the original method described in the first paragraph.

STRESS SINGULARITIES IN BONDED MATERIALS UNDER MECHANICAL AND THERMAL LOADING

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It is well known that stress singularities occur in solid bodies or even in viscous flows due to loading, structure and geometry of the body. An asymptotic expansion of the displacement or stress fields near the geometrical or structural peculiarities describes the singularities of the solution of the boundary or boundary-transmission problems. The structure of the expansion is strongly influenced by the mechanical and thermal loading and the structure of the material, e.g. isotropic or anisotropic or bonded dissimilar materials yield different expansions [5]. Unfortunately, there can be instabilities in the asymptotic expansion, that means logarithmic terms occur near critical angles and material parameters what leads to an increasing of the coefficients in the asymptotics for certain loads. This fact is known both in mechanics as the Sternberg-Koiter paradox for an elastic isotropic wedge [2] and in mathematics [3, 1]. The mathematical reason is, that a generalized eigenvalue problem generates the asymptotic expansion and that the changes of the algebraic and geometrical multiplicities of the corresponding eigenvalues are responsible for the logarithmic terms.

We analyse this situation for the Neumann-transmission problem for dissimilar isotropic materials, where the eigenvalue "one" with the rotational rigid motion as eigensolution is significant especially for different constant temperature fields in a coupled structure. We have developed a combination of MAPLE- and MATLAB-programs which find the critical angles and material parameters, where the expansion changes. We compare our results with the FEM-results from [4].

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FINITE ELEMENT APPROXIMATIONS OF VORTICITY SYSTEMS IN VISCOUS INCOMPRESSIBLE FLOW

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Initially a series of mathematical results obtained by the authors recently, concerning equivalence, existence and uniqueness for the velocity-vorticity formulations of the incompressible Navier-Stokes equations, in both two- and three-dimension space are recalled (see e.g. [1], [2], [4], [3], [5]). Next finite element methods for approximating such vorticity systems in the two-dimensional case are considered. The methods are based on an uncoupled solution method aimed at overcoming the lack of vorticity boundary conditions in general. Several standard Galerkin finite element schemes of arbitrary order are presented. Some of them lead to optimal convergence results in the framework of the linearized Stokes system, for both the stream function-vorticity and the velocity-vorticity formulations. Also some numerical results obtained for the former will be shown. Finally, new uncoupling techniques for the three-dimensional velocity-vorticity system are proposed and studied from the mathematical point of view. The study of corresponding optimally convergent finite element methods is underway, and new results in this connection could also be shown at the conference.

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A FINITE BOUNDARY-ELEMENT METHOD AS APPLIED TO DIRECT AND INVERSE SCATTERING FROM BURIED OBJECTS

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A boundary element method based on a rigorous integral formulation has been applied to the problem of scattering from cylindrical buried objects. Two kinds of geometrical configurations have been investigated, related to:

- cross-borehole tomography,
- radar detection (SAR, GPR, ...).

In the first case, where both the source and the receiver are embedded in the subsoil, the role of the air-soil interface has been neglected. The time-harmonic source is a 3D dipole antenna with arbitrary moment [2]. Thanks to a Fourier transform, the incident field can be written as a superposition of conical waves. It enables us to reduce the direct scattering problem to a set of uncoupled 2D problems. A peculiar attention is devoted to the singular part of the Green's function and its derivatives: it is systematically extracted and analytically integrated. Careful attention has also been paid to the branch points and the poles associated to guided waves or irregular frequencies.

In the second configuration, the air-soil interface is taken into account, as well as its roughness. The profile is assumed to be invariant with respect to the same direction as the buried cylinder. Since the surface is infinite, we have reduced the scattering problem to a bounded area by representing the incident field by a finite beam.

A first approach of the inverse scattering problem will be presented, using a simplified model of the cross-borehole configuration. The incident field is described by a s or p polarized cylindrical wave and the scatterers are perfectly conducting bodies. The method is based on an iterative conjugate-gradient algorithm. The computation of the gradient of the cost function, with respect to the displacements along given directions, is performed thanks to the Lorentz reciprocity relations [1]. This technique only requires the resolution of one more direct problem.

Numerical examples will be given for each problem.

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QUADRATURE TECHNIQUES FOR 3-D GALERKIN BEM

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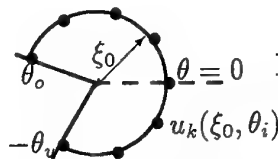
In our talk we will present efficient quadrature strategies for the approximation of the system matrix stemming from Galerkin discretizations of 3-d integral equations. These techniques can be applied to any kind of kernel function, surface approximation technique, and trial space. Only the subroutines which evaluates the kernel functions and the shape functions have to be modified. Furthermore this integration technique is relatively easy to implement since it can be tested isolated on simple examples.

STRESS CALCULATIONS AT INTERFACE-CORNERS(CRACKS) IN NONLINEAR DEFORMATION FIELDS

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Using material models on the basis of the flow theory of plasticity the asymptotic behaviour of solid mechanics solutions in crack tips, interface corners etc. strongly depends on the local realised load trajectory. For incrementally proportional load paths the equations determining the asymptotic fields are very simple ones [1]. The paper considers two dimensional statements in the neighbourhood of an interface corner consisting of two material ranges ($0 \leq \theta \leq \theta_o$ and $0 \geq \theta \geq -\theta_u$). At a distance of $\xi = \xi_o$ from the corner the finite element nodes of an regular net are established in a polar coordinate system of ξ and θ together with the displacements degree of freedom $u_k(\xi_o, \theta_i)$ (see picture).



Picture: Neighbourhood of an interface corner together with the finite element nodes

For formulations of this nonlinear (Plastic Flow Theory) statements the following boundary conditions are given:

- Vanishing normal and tangent stresses ($\sigma_{\theta\theta}, \sigma_{\xi\theta}$) at $\theta = \theta_o, -\theta_u$
- Continuity of normal and tangent stresses and displacements (u_ξ, u_θ) at $\theta = 0$

The main idea of the presented singular and nonsingular stress and deformation field calculation at interface corners characterizes an replacement of the corner neighbourhood ($\xi < \xi_0$) effect to the surrounding body ($\xi > \xi_0$) by introducing stiffness actions at $\xi = \xi_0$ which in usual manner can be assembled together with the other element stiffness matrices to the global stiffness matrix of the body. According to this there exists an interesting invariant stiffness dependence in corner and crack neighbourhoods. The applied technique allows extensions to nonproportional local load increments [1] simplifying the mathematical calculations for the presentation of stress and strain fields in this general case. All computations are made on modern parallel computers. Concrete examples shows the advantages of the presented approach.

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NONOVERLAPPING DOMAIN DECOMPOSITION WITH BEM AND FEM

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The Finite Element Method and the Boundary Element Method are two different structure analysis methods with a totally different numerical character. Therefore it makes no sense to couple these two structure analysis methods pointwise at the interface. A successful possibility is to work with a nonoverlapping domain decomposition method. If we want to analyze, for example, local effects in mechanical engineering, the region with high stress peaks and high stress gradients is described by the very precise approximation properties of the Boundary Element Method. In the residual domain we can work with classical finite elements. The kernel question is now: how do we realize the construction of the interface condition between the two subregions? The answer lies in defining mortar elements on the skeleton using a generalized compatibility condition in a weak sense. As a result, we have a symmetric positive definite operator for the whole structure so that this method can be incorporated in classical finite element software. In cooperation with G.C. Hsiao and W.L. Wendland we succeeded in formulating results for stability and asymptotic error estimation of the method. Besides that concrete results for mechanical engineering problems are obtained [1].

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BIORTHOGONAL WAVELET BASES AND MULTI-SCALE METHODS FOR INTEGRAL EQUATIONS

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The Boundary element method (BEM) offer an appropriate tool for the numerical solution of certain boundary value problems in engineering. A major drawback of BEM is the fact that the arising system matrices are densely populated. This effect hampers the discretization of realistic 3D problems with complex geometry. Like panel-clustering and multi-pole expansion, biorthogonal wavelet bases remedy this situation by approximating the discrete scheme efficiently. Multi-scale methods achieve this by approximating the system matrix relative to a biorthogonal wavelet basis by a sparse matrix. We propose a boundary element discretization for static or low frequency problems which is based on parametric surface representation. The surfaces are assumed to be only piecewise analytic and parametrized over quadrilateral surface (macro-)elements. Trial functions are supposed to be globally continuous and piecewise bilinear in each parameter domain.

We propose a biorthogonal wavelet basis with desired vanishing moments on each surface (macro-)element. In addition, this basis satisfies a stability condition so that the Galerkin wavelet method can be immediately preconditioned. The proposed basis has all desired properties achieving an asymptotically optimal balance between accuracy and efficiency. This means that we directly compute a sparse approximation of the system matrix causing only an error proportional the optimal error bound of the Galerkin discretization. This can be realized such that the total number of nonzero matrix coefficients increases only linearly with the total number of unknowns N . In order to compute the nonzero matrix coefficients directly, we propose an adaptive quadrature method, with the desired accuracy requiring totally $\mathcal{O}(N)$ floating point operations.

THE *HP* APPROXIMATION OF BOUNDARY LAYERS

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Boundary layers are rapidly varying components of the solution with support in a region around the boundary of the domain. They typically arise in the case of singularly perturbed PDEs, such as those for anisotropic heat flow and plate and shell models.

Approximating such solution components *uniformly* in terms of the parameter

tending to zero (i.e. the thickness in plate problems) is a difficult numerical problem. We will show how the hp version can be used to do this at an *exponentially* convergent rate. We will also address the case that both boundary layers and corner singularities are present. Our results provide the groundwork for assessing the efficiency of adaptive hp methods in resolving such components.

A POSTERIORI ERROR ESTIMATES IN THE ADAPTIVE FINITE ELEMENT METHOD OF LINES

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Adaptive approximation techniques for modeling various physical phenomena are usually based on a posteriori error estimates. The estimates developed recently in the finite element method of lines are simple, accurate, and cheap enough to be easily computed along with the approximate solution and practically applied to provide the optimal number and optimal distribution of space grid nodes.

This contribution is concerned with a posteriori error estimates and adaptive algorithms for the construction of a space grid for solving initial-boundary value problems for linear as well as nonlinear parabolic partial differential equations by the method of lines. Some numerical examples complement the theoretical considerations.

TOWARD ROBUST ADAPTIVE FINITE ELEMENT METHODS FOR PARTIAL DIFFERENTIAL VOLTERRA EQUATION PROBLEMS ARISING IN VISCOELASTICITY THEORY

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A brief introduction to how elliptic, parabolic and second-order hyperbolic partial differential equations with memory arise in modelling the response of linear viscoelastic materials is given. We focus on the elliptic-Volterra problem, and using the key assumption of fading memory—along with some comparison results from Volterra theory—we are able to by-pass the usual Gronwall lemma and give sharp data-stability estimates. These estimates also apply to a certain dual problem and this, coupled with the Galerkin orthogonality of the (space-time) finite element method, provides a route to a residual-based *a posteriori* Galerkin-error estimate. Such an estimate is derived and demonstrated numerically for a model problem in one space dimension.

A UNIFIED APPROACH TO *HP* FINITE ELEMENTS IN TETRAHEDRAL, PENTAHEDRAL AND HEXAHEDRAL DOMAINS

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Hybrid discretisation using a combination of structured and unstructured domains are a versatile way of dealing with complicated three-dimensional problems. Such an approach combines the simplicity and convenience of structured domains with the geometric flexibility of an unstructured discretisation. In two-dimensions, hybrid discretisation simply implies the use of triangular and rectangular domains however in three dimensions the hybrid strategy is more complex requiring the use of pentahedral domains, such as prisms and pyramids, as well as tetrahedrons and hexahedrons.

Structured rectangular and hexahedral domains have been used quite extensively in the *hp* finite element field [3, 1]. More recently an unstructured *hp* finite element approach has been developed for unsteady problems in fluid dynamics [2]. These two expansions can be constructed under one unified approach and the purpose of this paper is to present the *hp* finite element expansion for hybrid domains which encompasses the standard hexahedral expansion and the more recent tetrahedral expansion.

The construction of these bases employs a new co-ordinate system generated by the repeated application of a “rectangle to triangle” transformation. Building upon these new co-ordinate systems it is possible to develop expansions which are polynomials in both the co-ordinates as well as the standard Cartesian co-ordinates. Similar to the standard hexahedral expansion, the hybrid expansions are expressed as a generalised product in terms of the new local co-ordinates which means that automatic integration using Gaussian quadrature can be used to efficiently evaluate integrals. Efficiency in this type of operation is particularly important when dealing with unsteady problems where the “cost per time step” rather than the “setup cost” of the problem is dominant.

The construction of the new C^0 hybrid expansions will be motivated by developing orthogonal expansions within each of the hybrid domains. The extension to the C^0 expansions and its capability for *p*-type adaptivity will also be discussed.

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NATURAL CONVECTION

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In this paper, a boundary-domain integral method is presented for the solution of fluid motion problems which is based on the velocity-vorticity formulation of the Navier-Stokes equations. Since the pressure does not appear explicitly in the field equations, the well known difficulty connected with the computation of the pressure in incompressible fluid flow is avoided. To accelerate convergence the false transient approach is applied to the kinematic velocity equation. The Boussinesq approximation is considered to model the buoyancy effect in the momentum equation.

Due to the mixed parabolic-hyperbolic character of the governing diffusion-convective transport equations, the convection dominated flows suffer from numerical instabilities. To suppress such instabilities characteristic for the domain type numerical techniques some upwinding schemes have to be used. It is of main importance in the context of finding appropriate boundary-domain integral representation how to separate the partial-differential equation into a linear and nonlinear part. Based on various fundamental solutions of the corresponding linear differential operators different boundary-domain integral representations can be formulated. Parabolic diffusion, modified Helmholtz and diffusion-convective fundamental solutions are used.

Two sample cases are studied to demonstrate the applicability of the proposed numerical scheme based on boundary-domain integral formulation. The first one deals with standard natural convection in a closed cavity, while the second one represents the natural convection in a cylindrical annulus.

AN EFFICIENT INTEGRAL EQUATION METHOD FOR SCATTERING IN A ROUGH-SIDED WAVEGUIDE

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Boundary integral methods are needed for the accurate modelling of wave interactions in a rough-sided irregular waveguide. These result in coupled integral equations, however, whose treatment is highly computationally intensive. An efficient method is described to overcome this problem. The integral operator can be written formally as a sum of two components, corresponding to left- and right-going waves. Since most energy is forward scattered, one of these components has rapidly oscillating kernel, and can be treated as small. The solution of the integral operator can therefore be expanded as a series and truncated after one or two terms. Each term in this series describes multiple scattering and interaction between the left- and right-going waves, but is in Volterra form and is therefore highly convenient for numerical treatment. Computational examples will be presented to illustrate this approach.

NUMERICAL MODELLING OF THE REPLACEMENT OF THE TOTAL HIP PROTHESIS (THP)

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Alloarthroplasty is based on application of technical materials into living tissue. These materials are loaded by considerable periodical forces. It causes material fatigue of the THP and eventually leads to the fracture of the stem.

Besides the fractures of the stem of THP, the strain on the THP also leads to loosening of the components of THP as a result of the necrosis of the bone tissue, reaction of the tissue to the products of friction and atrophy of the bone.

Mathematical 2D model is based on contact problem of Signorini type with friction in linear elasticity. The numerical analysis of the problem is carried out and used algorithm is discussed. Proposed method is used for analysis of the real case of the patient with very complicated THP replacement.

ASPECTS OF THE LOCALIZATION ANALYSIS IN COMPUTATIONAL PLASTICITY

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This contribution is concerned with theoretical and numerical aspects of instability phenomena in multisurface elasto-plasticity which is the adequate constitutive framework for e.g. single crystal plasticity. To this end, the localization analysis for multisurface elasto-plasticity based on the additive decomposition of the geometrically linearized strain tensor is considered and the characteristic differences and similarities to the wellknown single surface case are highlighted. In the numerical part we subsequently discuss the computational setting of single crystal plasticity as the paradigm for multisurface elasto-plasticity. Finally, the numerical examples demonstrate the dramatic influence of the slip system orientation on the resulting localized failure mode of a single crystal compression panel. Summarizing, the lecture is organized as follows:

After introducing briefly the general setting of *multisurface* elasto-plasticity based on the additive decomposition of the geometrically linearized strain tensor we first investigate the conditions for *diffuse* failure which is characterized as the stationarity condition for the stress state. Thereby, the analysis relies on the simple structure of the corresponding elasto-plastic tangent operator in the form of a sum of rank 1 updates.

Next, the general localization or rather admissibility condition for the maintenance of a spatial discontinuity of the velocity gradient field is established. Based on this result we then discuss the condition for the onset of *continuous* localization for the case of *multisurface* elasto-plasticity. Thereby, the simple structure of the tangent operator carries over to the structure of the localization tensor and is thus frequently exploited. In particular, for multiple active constraints the determinant of the localization tensor is shown to be conveniently evaluated in terms of a new matrix containing the hardening moduli in a simple fashion. On the one hand, the critical hardening moduli, allowing for the onset of *continuous* localization, may be extracted from this matrix.

On the other hand, it turns out in the subsequent investigation that the condition for the onset of *discontinuous* localization is determined by negative spectral properties of this matrix. The analysis reveals the important result that in contrast to the *single surface* case *discontinuous* localization may precede *continuous* localization if *multiple* constraints are active.

In the numerical part we first discuss the computational setting of *single crystal* plasticity as a paradigm for *multisurface* elasto-plasticity. Thereby, the restriction to a geometrically linearized format allows for a particular simple and transparent integration algorithm. Finally, in the numerical examples we focus on the dramatic influence of the slip system orientation on the resulting localized failure mode and load carrying capacity of a *single crystal* compression panel.

ADDITIVE SCHWARZ METHODS FOR INTEGRAL EQUATIONS OF THE FIRST KIND

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We present additive Schwarz methods (two level and multilevel) for the h-version and the p-version of the boundary element method. Both weakly singular and hypersingular integral equations of the first kind are considered solving Dirichlet and Neumann problems for the Laplacian. For the p-version the condition number $\kappa(P)$ of the additive Schwarz operator P grows not worse than $\log^3 p$ where p is the degree of the polynomials used in the Galerkin boundary element schemes. For the corresponding multilevel method we have $\kappa(P)$ behave like $p \log^3 p$. For the h-version $\kappa(P)$ is bounded independently of the number of levels and the number of mesh points. Thus the additive Schwarz method as a parallel preconditioner in the CG method is also an efficient solver for boundary integral operators, which are non-local operators and lead to dense stiffness matrices. The additive Schwarz method can even be used to solve iteratively boundary element discretizations of indefinite integral equations arising from Helmholtz problems. Then the additive Schwarz operator is used as an efficient preconditioner for the GMRES, an iterative method of conjugate gradient type. The rate of convergence of the preconditioned GMRES turns out to be bounded for the h-version and grows as $\log^3 p$ for the p-version. Further we present a hierarchical basis method to derive an a-posteriori error estimate for the difference between the exact solution and the additive multilevel solution. Based on this estimate we introduce an Adaptive Multilevel Algorithm with easily computable local error indicators and direction control. The theoretical results are illustrated by numerical examples for the h and p versions of boundary integral equations on curves and surface pieces. Comments on the implementation of the algorithms are given.

**A UNIFORMLY CONVERGENT GALERKIN METHOD
ON A SHISHKIN MESH
FOR A CONVECTION-DIFFUSION PROBLEM**

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We analyze a Galerkin finite element method, which uses piecewise bilinears on a piecewise uniform mesh, for numerically solving a linear convection-dominated convection-diffusion problem in two dimensions. This method is shown to be convergent, uniformly in the perturbation parameter, of order $N^{-1} \ln N$ in a global energy norm and of order $N^{-1/2} \ln^{3/2} N$ pointwise near the outflow boundary, where the total number of mesh points is $O(N^2)$.

**FINITE ELEMENT METHODS
FOR CONVECTION-DIFFUSION PROBLEMS
USING EXPONENTIAL SPLINES ON TRIANGLES**

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A new family of Petrov-Galerkin finite element methods on triangular grids is constructed for singularly perturbed elliptic problems in two dimensions. It uses divergence-free trial functions that form a natural generalization of one-dimensional exponential trial functions. This family includes an improved version of the divergence-free finite element method used in the PLTMG code. Numerical results show that the new method is able to compute strikingly accurate solutions on coarse meshes.

An analysis of the use of Slotboom variables shows that they are theoretically unsatisfactory and explains why certain Petrov-Galerkin methods lose stability when generalized from one to two dimensions.

Full details are given in [1].

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MODELLING POLYMER PROCESSING USING THE NECKING NETWORK CONCEPT

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Many solid polymers neck when extended to large deformations. This remains true at high temperatures at which many solid phase deformation processes are performed, and some such processes are in effect a form of controlled necking. Polypropylene necks readily, and we have studied experimentally its large stretch behaviour at 150°C, a temperature relevant to processing regimes. The material is nonlinear viscoelastic. Previous attempts at modelling necking of polymers have been with glassy polymers at lower temperatures, and in these cases the mechanism of necking has been associated with rate-dependent components of the stress. In our case, however, we have observed that, as the temperature is increased and as a consequence rate dependence decreased, there is no lessening of the tendency to neck. We have therefore attributed the necking to an inherent feature of the polymer network. An established model of a polymer network due to [1] has just this feature, and has been incorporated into finite element schemes to model successfully the main features of necking polymer bodies. The original theory is for a hyperelastic material. In order to better represent the stress-strain behaviour of the polypropylene, a modification has been made to the model of [1] so that one of its parameters is assumed to be strain dependent. The resulting model is still elastic, but no longer hyperelastic. Although the time-dependence of the material is not included in the model, it produces realistic results. It has been incorporated into the ABAQUS finite element scheme and applied to various problems, including uniaxial and multiaxial stretching, and the production of oriented tube product by drawing the tube over a mandrel.

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DIFFERENTIAL-ALGEBRAIC SYSTEMS FROM PLASTICITY

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The change between elastic and plastic states are controlled by a plastic parameter different from zero only in the state of active loading. In the talk I will give a short overview about some loading and unloading criteria frequently used in engineering and computing practice. These are

the (classical) stress rate controlled criterion

the strain rate controlled criterion

the subdifferential approach

the semi-classical formulation

the Kuhn-Tucker formulation and

the formulation as nonlinear equation

Formal finite element discretizations of the resulting initial boundary value problems lead to different nonlinear (i.g. non-smooth) differential-algebraic systems corresponding to classical index 2 differential-algebraic equations. A brief discussion of the numerical solution by means of implicit time integration and nested linearization techniques conclude the talk.

COVARIANT MIXED FINITE ELEMENTS

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We develop and analyse mixed finite elements approximation for an elliptic problem described on a surface Ω of \mathbb{R}^3 .

Before writing the equations, let us specify some notations (Einstein's summation convention will be used). Let $(y_1, y_2) \in \omega \subset \mathbb{R}^2$ be a curvilinear coordinates system for the surface: $\Omega = \varphi(\omega)$.

If u is a function defined on Ω , the covariant components of its gradient are the two quantities given by $\partial_\alpha u = \partial u / \partial y_\alpha$; if s is a vector field defined on Ω , the β -th covariant derivative of the α -th contravariant components is given by

$$D_\beta s^\alpha = \partial_\beta s^\alpha + \Gamma_{\beta\gamma}^\alpha s^\gamma$$

where the $\Gamma_{\beta\gamma}^\alpha$ are the Christoffel symbols of the surface. The covariant divergence of \mathbf{s} is the function $Div \mathbf{s} = D_\alpha s^\alpha$; we have : $Div \mathbf{s} = \frac{1}{\sqrt{a}} \partial_\alpha (\sqrt{a} s^\alpha)$ where a is such that the area element on the surface is $d\Omega = \sqrt{a} d\omega$.

We consider the Dirichlet problem

$$\begin{cases} Div \mathbf{s} + f = 0 & \text{on } \Omega \\ \mathbf{s} = \mathbf{grad} u & \text{on } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases} \quad (1)$$

(u is solution of the Beltrami equation : $-\frac{1}{\sqrt{a}} \sum_{i=1,2} \partial_i (\sqrt{a} \partial_i u) = f$).

The covariant mixed method is based of the following formulation of Problem (1) : find $\mathbf{s} \in W$ and $u \in M$ solutions of

$$\begin{cases} \forall \mathbf{r} \in W, & \int_{\Omega} a_{\alpha\beta} s^\alpha r^\beta d\Omega + \int_{\Omega} u D_\alpha r^\alpha d\Omega = 0 \\ \forall v \in M, & \int_{\Omega} v D_\alpha s^\alpha d\Omega = - \int_{\Omega} f v d\Omega \end{cases} \quad (2)$$

where $M = L^2(\Omega)$ and $W = H(Div; \Omega)$ are functional spaces defined on the differential manifold Ω and where the $a_{\alpha\beta}$ are the covariant components of the fundamental tensor.

Compatible finite dimensional subspaces W_h and M_h would be proposed for the finite element approximation of (2).

ON THE CONVERGENCE OF NONCONFORMING STREAMLINE DIFFUSION METHODS APPLIED TO CONVECTION DIFFUSION PROBLEMS

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The streamline-diffusion method (SDFEM) for the solution of convection-diffusion problems has been successfully implemented with the use of conforming finite element spaces. Proposed first by Hughes [1] the mathematical analysis of the SDFEM starts in [3] and nowadays its convergence properties are well-understood in the conforming case [2], [4], [5], [6], [7].

For computational fluid dynamics applications, finite element methods of nonconforming type are more attractive than those of conforming type since nonconforming elements more easily fulfill the discrete version of the Babuška-Brezzi condition. When switching from a conforming to a nonconforming SDFEM, one loses the Galerkin orthogonality and has to consider an additional consistency error. For the standard coercive discrete bilinear form it will be shown that the consistency error is not of optimal order, uniformly with respect to the perturbation parameter ε . The main

objective of this paper is to present several nonconforming streamline-diffusion finite element discretizations for the solution of the boundary value problem

$$-\varepsilon \Delta u + b \cdot \nabla u + cu = f \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \Gamma, \quad (1)$$

and to discuss the convergence properties both from theoretical and numerical point of view.

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ADDITIVE SCHWARZ ALGORITHMS IN THE BOUNDARY ELEMENT METHOD

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We study 2-level and multilevel additive Schwarz methods as preconditioners to solve iteratively systems of equations arising from the Galerkin discretisation of weakly singular and hypersingular integral equations. Both the h - and p -versions of the Galerkin scheme are considered. We prove that the condition numbers of the preconditioned systems are bounded independently of the mesh size and the number of levels in the case of the h -version, and bounded by $1 + \log^3 p$ (resp. $p(1 + \log^3 p)$) for the 2-level (resp. multilevel) method in the case of the p -version, where p is the polynomial degree. Thus we show that additive Schwarz methods which were originally designed for differential operators are also efficient solvers for integral operators, even though integral operators are non-local.

ALGEBRAIC MULTIGRID FOR SOLIDS, PLATES AND SHELLS

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An algebraic multigrid algorithm for symmetric, positive definite linear systems is developed based on the concept of prolongation by smoothed aggregation and minimization of energy of coarse-space basis functions. Coarse levels are generated automatically. We present a set of requirements motivated heuristically by a convergence theory. The algorithm then attempts to satisfy the requirements. Input to the method are the coefficient matrix and zero energy modes, which are determined from nodal coordinates and knowledge of the differential equation. Efficiency of the resulting algorithm is demonstrated by computational results on real world problems from solid elasticity, plate bending, and shells.

**WAVELET-LIKE HB FINITE ELEMENT SPACE
DECOMPOSITIONS MULTILEVEL ITERATIVE METHODS
BASED ON STABLE WAVELET-LIKE HIERARCHICAL BASIS
FINITE ELEMENT SPACE DECOMPOSITIONS**

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In this talk we will present multilevel iterative methods for solving second order elliptic problems that exploit H^1 -stable modifications of the classical hierarchical basis (or HB) finite element space decompositions.

The stable wavelet-like modification of the classical HB decomposition, as proposed in Vassilevski and Wang (1995), is based on accurate approximations Q_k^a to the exact L^2 -projection operators $Q_k : L^2(\Omega) \rightarrow V_k$ such that

$$\|(Q_k^a - Q_k)v\|_0 \leq \tau \|Q_k v\|_0 \quad \text{for any } v \in L^2(\Omega).$$

The accuracy $\tau > 0$ is assumed sufficiently small, but independent of $h = h_J$ - the finest mesh size. Here, V_k is the k th level finite element discretization space.

We will present in the talk more details on the constructions of proper approximate L^2 -projections Q_k^a that lead to computationally feasible coordinate spaces $V_k^1 = (I - Q_{k-1}^a)(I_k - I_{k-1})V$ in the direct multilevel space decomposition $V = V_0 \oplus V_1^1 \oplus \dots \oplus V_J^1$. Here I_k is the k th level nodal interpolation operator and $V = V_J$ is the conforming finite element space at the finest (J th) level grid.

Based on the above H^1 -stable direct multilevel decomposition one can construct classical iterative preconditioning schemes of Gauss-Seidel (or multiplicative) type or Jacobi (or additive) type for solving the, associated with the given bilinear form $a(.,.)$ and V_J , discretization problems that are optimal in the usual sense.

These schemes are in close relation with the multigrid, the well known BPX-method as well as with the algebraic multilevel methods.

The case of problems with discontinuous coefficients will be also outlined and it is based on a standard domain decomposition strategy.

TRANSFER OF BOUNDARY CONDITIONS FOR PARTIAL DIFFERENTIAL EQUATIONS

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The method of transfer of boundary conditions yields a universal frame into which most methods for solving boundary value problems for ordinary differential equations (as the shooting method, the invariant imbedding method etc.) can be included.

The purpose of this contribution is to show some possibilities how to extend this idea to some particular two-dimensional problems.

NUMERICAL SIMULATION OF THE VISCOUS SINTERING OF POROUS GLASS USING AN INTEGRAL FORMULATION FOR THE REPRESENTATIVE PERIODIC UNIT CELL

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A mathematical model and the obtained numerical results are presented to simulate the viscous sintering phenomenon, i.e. the process that occurs (for example) during the densification of a porous glass heated to such a high temperature that it becomes a viscous fluid. The mathematical approach consists of simulating the shrinkage of a two-dimensional unit cell which is in some sense representative for the porous glass. Hence it is assumed that the microstructure of the glass can be described by a periodic continuation in two directions of this unit cell.

The viscous sintering of this porous glass is mathematically modeled as a two-dimensional Stokes fluid of a lattice of equal (unit) cells with holes inside. Therefore a mathematical formulation is developed in terms of an integral equation based on Green's formulation, whereby the fundamental solution is used that represents the flow due to a periodic lattice of point forces, cf. [1]. The numerical simulation is carried out by solving the governing integral equations for a fixed domain through a Boundary Element Method (BEM). The resulting velocity field then determines an approximate geometry at a next time level which is obtained by an implicit integration method (BDF), cf. [3].

Applying this model it is possible to obtain quite a few theoretical insights of the viscous sintering process with respect to both pore size and pore distribution of the porous glass. In particular this model is able to examine the consequences of microstructure on the evolution of the pore size distribution. The major finding is that the pores vanish in order of size one after another; the smallest pores first,

followed by the larger ones. Moreover it is shown that pores with concave boundary parts may grow initially before they start shrinking at a later time stage, cf. [2].

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ERROR BOUNDS FOR FINITE-ELEMENT METHODS

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Several recent studies have given methods for estimating the error of finite-element solutions to boundary-value problems, with the aim of achieving a specified accuracy by mesh refinement (for example [6, 2]). Practical methods should be reasonably economical and not too pessimistic, and should give correct asymptotic results as $h \rightarrow 0$. In some cases it may also be of interest to compute strict bounds on the solution, for example to ensure that safety limits are not exceeded. This is more difficult than obtaining an asymptotic error estimate, but variational results can be used to produce upper and lower bounds on the solution in certain cases ([3, 1]). If the bounds are satisfactory there may be no need to refine the mesh.

This paper gives some methods for bounds in 1D and 2D, with numerical examples. To obtain good results it is necessary to consider smoothing and recovery techniques, in order to make use of the best local accuracy available (cf. [4]). This is not altogether straightforward, and the calculations can be rather lengthy in 2D. For strongly elliptic problems the solutions can be related to monotonicity results, but these require a high degree of smoothness, and we are more concerned with error bounds for solutions of low continuity.

Bounds can be obtained either for point values or for other combinations of solution values. Results are given for linear problems, but the methods can be extended to nonlinear problems if we have enough information about the operator.

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NUMERICAL SIMULATION OF NON-AXISYMMETRIC PRESSURE DRIVEN THERMOFORMING

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In thermoforming thin flat polymeric sheets are deformed in an oven environment into rigid moulds (to which it freezes to on contact) to form container type structures. In this paper we describe our efforts to model this process “robustly” and “efficiently” in the case of a pressure driven forcing action, isothermal conditions and a Mooney-Rivlin elastic membrane model. This briefly involves the following.

With a total Lagrangian formulation and with Ω denoting the region of the undeformed mid-surface the problem is to determine, for each value of the applied pressure P , the displacement field $\underline{u} = (u_1, u_2, u_3)^T$, $u_i = u_i(x_1, x_2)$ and the non-contact and non-contact regions Ω_{free} and Ω/Ω_{free} such that the boundary conditions, the total sticking assumption (for the contact with the mould) and the quasi-static equilibrium requirement are satisfied. The main implementation difficulties are thus that of adequately determining how Ω_{free} varies with P and of robustly and efficiently solving the non-linear equations to obtain the finite element displacement field. In our approach we use a piecewise linear finite element discretization on meshes which adaptively change as Ω_{free} changes together with continuation techniques and Newton’s method to reliably generate solutions to the non-linear systems which are encountered during the procedure. Some results with the approach are presented. We also discuss difficulties that are being encountered and consider future work that has to be undertaken to extend the present model to design tool capability.

RECENT DEVELOPMENTS IN BOUNDARY ELEMENT METHODS

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This lecture is a survey on new results in boundary element methods which mostly have been accomplished during the six years support of the Priority Research Programme 'Boundary Element Methods' of the German Research Foundation DFG. The lecture will focus on the following topics:

- Coupling of finite and boundary elements with traditional coupling, weak coupling and Trefftz elements, applications with nonlinear Newton potentials and for nonlinear problems involving nonlocal coupling with farfields.
- Domain decomposition with boundary elements, the formulation of nonoverlapping Schwarz methods and efficient solution procedures via preconditioned iterative methods; window techniques and overlapping Schwarz methods.
- Clustering, multipoles and wavelets.
- Numerical integration in connection with regularization techniques and special Gauß integration, applications to the cluster methods.
- Higher order and recovery methods and the evaluation of derivatives up to the boundary.
- Adaptivity; and error and stability analysis on unstructured as well as on structured grids.
- Transient problems.

The reports on these results will be published soon in [1].

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OPTI, A UNIVERSAL TOOL FOR OPTIMIZATION PROCEDURES IN CONNECTION WITH FINITE ELEMENT CALCULATIONS

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The finite element method provides a powerful tool for many applications in engineering sciences. In general, the commercial or educational finite element software products allow the straightforward calculation of some properties for a given model and related boundary conditions. In many cases, however, the model is not explicitly given but required to match with prescribed demands in industrial applications. Therefore, a new software package has been developed, which allows the implementation of optimization algorithms for different applications. The method is based on a general least squares approach for the relevant quantities. It uses a combination of two strategies, the gradient method and linearization of the fitting function, which allows an efficient search in parameter space. Via a software interface the user can decide which quantity should be fitted. This is demonstrated by two different examples. In a first example the geometric structure of a gas lighter is parametrized by a suitable model. A gas lighter is used as a firing equipment to ignite a gas mixture. The parameters of this model are optimized by the present procedure in order to ensure a prescribed temperature at a given small time. The gas lighter consists of a ceramics, on which an AC-voltage is applied. Due to the shape of the material, the resulting current produces a Joule heating so that we are dealing with a coupled electric thermal problem. The corresponding transient temperature field is calculated with the finite element method, in which radiation boundary conditions are taken into account. The capabilities of OPTI are demonstrated by a second example originating from the field of music. The sound generation of brass tubes by external vibration excitation is dictated by the corresponding frequency spectrum of the involved harmonic overtones. These eigenfrequencies can be calculated with the finite element method. For a given geometry and material property, the eigenfrequencies are mainly dominated by the length and thickness of the brass tubes. These quantities are optimized in order to manufacture one complete octave of equi-tempered tubes.

MIXED FINITE ELEMENT METHODS FOR MODELING MULTIPHASE FLOW IN POROUS MEDIA

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In this presentation we summarize some of the issues and problems associated with the modeling of multicomponent multiphase flow and transport in porous media. In particular we discuss a compositional model which involves the transport of a large number of chemical species in one to four fluid phases interacting with multiple solid mineral phases making up the permeable media. These problems arise in both petroleum engineering and environmental science. An important application of the latter is the modeling of dense non-aqueous phase liquids (DNAPL) contamination. Examples of these contaminants are chlorinated organic solvents, e.g. TCE and PCE.

DNAPLs pose a great challenge for cleanup in the subsurface since these organic contaminants have low liquid viscosities, low interfacial tensions with water, high volatilities, low absolute solubilities, low degradabilities, and are difficult to detect. Generally not all of the DNAPL can be pumped or flushed out with water or any other fluid with which it is immiscible. Thus numerical simulation is essential in developing special remediation strategies.

We present a numerical formulation based on mixed finite element methods with upstream weighting for these problems. We will describe how nonmatching grids can be applied for treating faults and source and sink terms. Numerical results for a two phase case are presented.

A MIXED DYNAMIC FINITE ELEMENT ANALYSIS OF HYPERELASTIC MATERIALS

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The paper is concerned with the dynamic analysis of rubber-like materials so as to compute their response to impact loading. A mixed variational principle is used to develop a finite element program for 3-D dynamic behaviour of nearly incompressible materials.

This kind of material is very difficult to study. The main difficulties are due to many facts: these materials are non linear and hyperelastic, they can have very large strains (up to 50% in compression and more that 500% in traction), they are incompressible or nearly incompressible and very sensitive to the strain rate. The con-

struction of the constitutive law have been done from experimental results performed on a sample for different values of the strain rate . A Hart-Smith law have been choosen to describe the internal energy and to obtain the constitutive relations. A Lagrange multiplier is introduced to take in account the incompressibility condition.

The finite element implementation is obtained with the virtual work principle, written in the total Lagrangian formulation. Unfortunately, this principle cannot be directly used for any incompressible continuum because the stress is dependent on the multiplier which is unknown in the constitutive law. We have therefore to use a penalty method to write this incompressibility condition. The problem is then solved with a mixed variational formulation. The mixed method have been often used in static analysis of rubber-like materials. In case of dynamic analysis a direct implicit finite element method can also be used, but the numerical results on the stresses give many oscillations. A dynamic mixed f.e. is here developped, it seems for the first time. It is shown that oscillations provide from the method used to write the incompressibility condition. A prediction-correction process is introduced to eliminate these oscillations. Numerical results show that our method is accurate.

A TRI - TREE ADAPTIVE REFINEMENT-RECOARSEMENT FINITE ELEMENT MULTIGRID ALGORITHM FOR THE NAVIER - STOKES EQUATIONS

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Local recoarsements of finite element grids for solving the Navier - Stokes equations are investigated. The recoarsement algorithm is based on the hierachic Tri - Tree multigrid generation algorithm and computes a local Tri - Tree Element Reynolds number. Previous investigations show that the Element Reynolds number is critical for convergence of the linear CGSTAB equation solver. A necessary condition for convergence is found to be that the Element Reynolds number is less than 10.

The Tri - Tree multigrid solution algorithm starts by solving the equations for a low Reynolds number for a coarse grid. Solutions for higher Reunolds numbers are obtained by gradually increasing the velocity boundary conditions while refining the grid correspondingly to satisfy the element Reynolds criterion. As the global Reynolds number is increasing, the non linear convection moves in space. The recoarsement algorithm is then making the grid coarser at locations where the previous fine grid resolution is no longer required.

Finite element grid refinements have demonstrated advantageous properties for both stabilizing the Navier - Stokes differential equation system and for resolving the solution of the equations at locations of high convection and gradients. These properties are extremely desirable, especially in aerodynamics where shocks are frequently appearing. In fluid flow, grid refinements are necessary to describe convection phenomena satisfactorily.

As grid refinements have been considered as a necessity in order to obtain an accurate solution of the equation system, little attention has been paid to grid re-

coarsements. The underlying philosophy of grid recoarsements is that the grid should not be finer than strictly necessary to describe the solution adequately. The effect of grid recoarsements can give considerable savings in both computer runtime as well as in computer storage.

The Element Reynolds number is applied to indicate where the grid is both coarser and finer than necessary to obtain a satisfactory solution. Those elements which have an Element Reynolds number less than a limit are recoarsed and elements with an Element Reynolds number greater than the same limit are refined. These element adjustments will then ensure that all elements have the largest size possible with an Element Reynolds number less than the predefined limit. The refinement - recoarsement algorithm is based on the Tri - Tree multigrid generation method.

The efficiency of the recoarsement algorithm which has been demonstrated for the present non linear cavity problem is expected to be even more profitable for time dependent problems. When studying moving shocks, the grid can be refined in the vicinity of the shocks and the grid can then be cleaned up by recoarsening of the grid after the shock has passed.

MULTI-GRID METHODS FOR POROUS MEDIA FLOW

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Multi-grid methods are well known as fast solvers for large systems of equations. Originating as fast Poisson solvers, in the last decade multi-grid methods have been developed for numerous application problems such as incompressible and compressible free flows and others. The application of multi-grid methods for porous media problems, however, is not so common in practice by several reasons. Porous media flow problems typically mean strongly jumping coefficients which are stochastically distributed and, in the unsaturated case, marching fronts and free boundaries. All this makes a coarse-grid approximation very difficult.

In the present talk we discuss handling of the multi-grid method in the presence of stochastically jumping coefficients for several porous media flow problems. The applicability of the discussed approaches is shown by experimental results.

NUMERICAL SIMULATION OF VISCOUS FINGERING USING B-SPLINE BOUNDARY ELEMENTS

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The phenomenon of viscous fingering in a porous medium refers to the onset and evolution of instabilities that occur in the displacement of the interface between two immiscible fluids with different viscosities. This fingering instability appears when a fluid of higher viscosity is penetrated by another fluid of lower viscosity; in this case, the interface between the two fluids is unstable to perturbations of certain wave lengths, and long fingers of the less viscous fluid penetrate the more viscous one.

The mathematical modelling of viscous fingering problems is generally carried out by using a potential model representation. Since the interface between the two fluids experiences large deformations, and the correct determination of its shape is of foremost importance, boundary integral representations have become popular in this field [2]. Viscous fingering models also possess similarities with other potential models for processes like crystal growth (see e.g. [3]).

This paper presents a numerical scheme, based on uniform cubic B-spline boundary elements, to simulate one-phase viscous fingering in Hele-Shaw cells. The one-phase approximation means that the viscosity of the less viscous fluid is so small that it may be ignored. The internal surface of the high viscous fluid is deformed by surface tension, and so it is important that the shape of this interface is properly modelled in order that the local curvature at each interface point may be accurately evaluated. For this, the BEM model employs uniform cubic B-splines following Cabral *et al.* [1]. The advantage of using this approximation is that it provides a high degree of continuity between elements.

Results will be presented for the cases of fingers growing in a channel and of radial fingering. The results obtained attest that the numerical model is well suited for handling the evolution of moving surfaces.

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NUMERICAL ANALYSIS OF SINGULARITIES IN 2-D LINEAR ELASTOSTATICS BY THE MODIFIED STEKLOV METHOD IN CONJUNCTION WITH P-FEM.

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In many important problems of structural mechanics the exact solution may be singular at one or more points. The solution for the linear elasticity problem in two dimensions (2-D) in the vicinity of a singular point can be expanded in the form:

$$\vec{u} = \sum_{i=1}^I \sum_{m=0}^M C_{im} * r^{\alpha_i} * \ln^m r \vec{f}_{im}(\theta) + \vec{u}^*$$

where \vec{u}^* is smoother than the terms in the sum, C_{im} are the generalized stress intensity factors (GSIFs), α_i and $\vec{f}_{im}(\theta)$ are eigenpairs which depend on the differential operator and the boundary conditions. The determination of these eigenpairs is an essential step towards reliable computation of the GSIFs, which are of great practical importance because failure theories directly or indirectly involve these coefficients. At present, the possibility to evaluate the eigenpairs and the GSIFs in a 2-D domain, especially at multi-material interfaces and in anisotropic materials, is very limited.

A new numerical method based on the "modified Steklov" formulation, for the computation of the eigenpairs resulting from singularities due to corners, abrupt changes in material properties and boundary conditions, is presented [1]. Specifically, the Steklov eigenvalue weak form is cast in the following form:

$$\text{Seek } \alpha \in \mathcal{C}, \vec{0} \neq \vec{u} \in H^1(\Omega_R) \times H^1(\Omega_R) \text{ satisfying}$$

$$\mathcal{B}(\vec{u}, \vec{v}) + \sum_{i=1}^2 \mathcal{M}_i(\vec{u}, \vec{v}) - \mathcal{N}(\vec{u}, \vec{v}) = \alpha \mathcal{M}_R(\vec{u}, \vec{v}), \quad \forall \vec{v} \in H^1(\Omega_R) \times H^1(\Omega_R).$$

where \mathcal{B} , \mathcal{M}_i , \mathcal{N} , \mathcal{M}_R are sesquilinear forms which will be explicitly presented. The formulation is finite element-oriented, applicable to multi-material domains, and uses the special features of p-extensions (with hierarchic shape functions).

The efficiency, robustness, and accuracy of the method is demonstrated by three numerical examples: A 90° corner of an isotropic material with one edge clamped and the other traction free, a graphite-epoxy interface meeting at an edge, and a composite body consisting of two dissimilar isotropic, elastic wedges, perfectly bonded along their interfaces. The numerical results are compared with the analytical solutions, which indicate that the computed values converge strongly, are accurate and inexpensive from both the computational point of view and the point of view of human time needed for input preparation.

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POINTWISE STRESS EXTRACTION BY THE COMPLEMENTARY ENERGY PRINCIPLE FROM *P*-VERSION FE SOLUTIONS.

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An accurate method for computing the pointwise stresses in the theory of linear elasticity in two-dimensions is presented and demonstrated on two example problems. The method, denoted by *SEC* (Stress Extraction by Complementary principle), is based on the complementary energy principle applied over a local domain in the post-processing phase in conjunction with the *p*-version FEM based on the displacement formulation.

It is demonstrated that the performance of the SEC method is *independent* of the Poisson's ratio, therefore suitable for nearly incompressible materials, and that accurate and reliable pointwise stresses can be extracted in the interior and on the boundaries of a domain. Also, the SEC method is applicable to points where stress singularities exist [2] (as crack tips, reentrant corners and multi-material interfaces) for the computation of the *generalized stress intensity factors*. Numerical examples are presented [1] in which accurate pointwise stresses are obtained, and the rate of convergence is at least as fast as that of the error measured in energy norm.

A short outline of the method: Assume that the stresses at a specific point in a domain Ω are of interest, and that the displacements in Ω are already computed using the usual displacement formulation. A localized sub-domain around that point of interest is considered, denoted by Ω_R , over which the complementary weak formulation for the elasticity problem is formulated:

$$\begin{aligned} \text{Seek } \boldsymbol{\sigma} \in \Sigma(\Omega_R) \quad \text{such that} \quad \forall \boldsymbol{\sigma}_o \in \Sigma(\Omega_R): \\ \iint_{\Omega_R} (\sigma_{11}, \sigma_{22}, \sigma_{12}) [E]^{-1} \begin{Bmatrix} (\sigma_{11})_o \\ (\sigma_{22})_o \\ (\sigma_{12})_o \end{Bmatrix} d\Omega = \int_{\partial\Omega_R} \mathbf{u}^T \cdot (\boldsymbol{\sigma} \cdot \mathbf{n}) ds. \end{aligned} \quad (1)$$

Here $\Sigma(\Omega_R)$ is the statically admissible space. We discretise the complementary weak form over Ω_R by choosing a sequence of finite dimensional subspaces $\Sigma^N(\Omega_R) \subset \Sigma(\Omega_R)$ (N denoting the dimension). Any $\boldsymbol{\sigma}$ which belongs to $\Sigma^N(\Omega_R)$ can be written in the form $\boldsymbol{\sigma} = \sum_{i=1}^N a_i \mathbf{f}_i$, where \mathbf{f}_i are smooth vector functions derived from an Airy stress function. On $\partial\Omega_R$ the FE solution obtained by the displacement formulation (\mathbf{u}^{FE}) is prescribed and the discretised complementary weak form is solved thus obtaining the pointwise stresses.

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PARALLEL ALTERNATING-TYPE ITERATIVE METHODS

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We consider parallel alternating-type iterative methods for solving discrete Dirichlet problems and discrete periodic problems involving the Poisson equation on rectangular domains. Examples of alternating-type methods include alternating direction implicit methods (ADI methods) for discrete Dirichlet problems and implicit unsymmetric SOR methods (USSOR methods) for discrete periodic problems. It can be shown that under certain conditions one can carry out m^2 single iterations of an alternating-type method using different pairs of iteration parameters and, after combining the results, obtain the same result as would be obtained by carrying out m iterations of the method in sequence, again with varying iteration parameters. Thus there is a potential saving of a factor of m in the wall clock time. The procedure is based on the use of a partial fraction representation of a rational function of two variables.

UPDATING OF LARGE SIZE FINITE ELEMENT MODELS BY EXPERIMENTAL MODAL DATA AND INVERSE PROBLEMS

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The progress in dynamic analysis of real engineering structures represented by a very large number of degrees of freedom FE model and a set of measurement data needs special consideration in procedures and algorithms that improve model quality. Updating methods, using both measurement and FEA results, capable of handling practical problems have to be robust and economical. Therefore a suitable procedure has to avoid repeated reassembling and decomposition of system matrices for sake of solution time and storage capacity. Under the assumption of compact structure and sufficient approximation of mode shapes in the initial model a fast and efficient algorithm is presented in the paper and validated on a real, complicated engineering structure. A utilisation of substructure/superelement technique has been shown possible. This paper is focused on very large compact FE models only. For such large size dynamic FE models the number of degrees of freedom is much greater than number of pick ups for measurement. Hence equations for updating are underdetermined equations. Since these equations cannot be satisfied exactly, we may attempt to satisfy them as best as we can. That is to minimise the residual vector using the Euclidean (or least square) norm.

From the linearisation of equations it is obvious, that an iterative procedure is required for updating the FE model. Consequently, after each updating step we get the changes by solving an eigenvalue problem. With repeated solution of the eigenvalue problem including changes of mass and stiffness matrix, new sets of modal parameters are calculated. It is most effective to include the updating algorithm described in the paper into a special subspace iteration technique for solving the eigenvalue problem within a FEA code. In case of stiffness changes it is necessary to keep the original stiffness matrix unchanged within the iteration algorithm. The time consuming decomposition in every updating step can be avoided in this way. In the paper it is shown how to do so. In each update iteration stage only few steps for solving of the changed eigenvalue problem are necessary (2-3 steps). Alterations in masses are generally easier to realise in constructive design or experiment than alterations in stiffness. The method presented fulfils both tasks of updating constructive changes (stiffness and mass distribution) that lead to definite frequencies and mode shapes of structure and improvement of the mathematical model for a dynamic analysis in a certain frequency range. Implementation of this algorithm into the commercial FE-code COSAR has shown that for large FE models good results can be obtained with a relative small amount of additional computational work. The presented algorithm can be the basis for optimisation procedures. In optimisation algorithms an efficient solution of the update problem is in particular for large FE models, of great importance. Thus the method described in the present paper is suitable to perform in that way.

FEM WITH SPLINE INTERPOLATION FUNCTIONS IN NONLINEAR ANALYSIS OF STRUCTURES

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In this paper the nonlinear finite element analysis with the help of spline functions in structural engineering is introduced. The solution techniques for three different problems in structural analysis are presented. The first problem is the local stability analysis of plate groups. The spline function and triangular function are taken to describe the out-of-plane deflecting of plates along transverse and longitudinal directions, respectively. The finite element equations for one plate and plate group can then be established. The bifurcation loads of plate groups can be solved. The influence of residual stresses is considered in analysis. The second problem is the ultimate strength of plane beam-columns. The spline function is taken as the interpolation function of beam-columns. The load-deflection procedures and ultimate strength of beam-columns can be satisfactorily solved from the finite element equations with the help of N-R iterative techniques. All initial imperfections, including initial deflections, initial eccentricities and residual stresses, are taken into account. The third problem is the nonlinearly static and dynamic analysis of spatial cables. The spline function is taken as the interpolation function of cable element in all three directions. The numerical examples show that such cable element has higher accuracy than the elements with linear or curve interpolation functions. The lack of the spline finite element method is also pointed out in the paper. In 2D full potential flow is considered as a numerical example.

ON MATHEMATICAL ANALYSIS OF SPR

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Among derivative recovery techniques of the finite element method, the Superconvergence Patch Recovery (SPR) procedure by Zienkiewicz and Zhu is very promising. If the pollution is not present or is properly controlled, SPR performs very well in the interior of the domain even when the mesh is distorted so that the natural superconvergence points are lost. Moreover, SPR is effective for both triangle and quadrilateral elements of any order. The computational expense of this local least squares fitting procedure over an element patch is only a very small fraction of the entire computing time. Since its effectiveness and simplicity, SPR has quickly established itself in engineering community. However, regardless of its success in practical computations, very little work has been done concerning the theoretical justification.

In this work, a mathematical analysis for SPR is presented. It is shown that under certain conditions, SPR results in local superconvergence recovery not only at a nodal assembly point, but also on the whole element patch. In some situation, superconvergent recovery is obtained at a nodal assembly point even when the surrounding sampling points are not natural superconvergence points.

A surprising observation from numerical tests of SPR is ultraconvergence (i.e., two orders higher) based on the superconvergent data at the Gaussian points. An $O(h^4)$ convergence rate has been reported for the recovered derivative at the internal nodal points when quadratic elements and uniform meshes in the element patch are used. Note that if a more sophisticated recovery technique were applied, $O(h^4)$ would be of no surprise. The point is that only a simple local least squares fitting is applied here. In the one-dimensional setting, this astonishing phenomenon has been fully explained for a class of two-point boundary value problems. It is shown that the recovery procedure will result in ultraconvergent internal nodal recovery when locally uniform meshes and even order elements are used. In the two dimensional setting, only the tensor product element for the Laplace equation is considered. Now the situation is more complicated since domains with non-smooth boundaries may lead to singular solutions. If this happens, local mesh refinement is applied such that global error in a negative norm is two order higher than that of the energy norm. Then it can be proved that SPR is able to produce an ultraconvergence recovery for the derivative at an interior nodal point if the adjacent four rectangular elements (the element patch) are uniform and an even order finite element space is used.

INTEGRAL EQUATION METHOD FOR ELECTROMAGNETIC SCATTERING BY AN INHOMOGENEOUS LAYER ON A PERFECTLY CONDUCTING PLATE

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The scattering problem of time harmonic electromagnetic plane waves by an inhomogeneous conducting or dielectric layer on a perfectly conducting plate is considered. The magnetic permeability is assumed to be a fixed positive constant in the media: within the layer the permittivity and conductivity are assumed constant in one coordinate direction parallel to the plate (so that the problem is two-dimensional) but are allowed to vary in an arbitrary bounded measurable way in the other two directions. We are restricted to the case of TE polarization, so that the problem is modelled by the reduced wave equation with variable index of refraction in the layer and a Dirichlet condition on the plate. To complete the problem formulation a radiation condition on the scattered field component is introduced, a generalisation of the Rayleigh expansion condition for diffraction gratings. The problem is reformulated as a Lipmann-Schwinger integral equation over the layer. Conditions on the variation of conductivity and permittivity in the layer are given which ensure uniqueness of solution (non-existence of pure surface waves). General results on the solvability of integral equations on unbounded domains are used to establish existence of solution, continuous dependence in a weighted norm of the solution on the given data, and stability and convergence of a finite element collocation solution scheme. The weighted norm permits the scattered field to grow algebraically with distance from the boundary. An example shows that this growth can be achieved by a suitable permittivity variation within the layer.

A POSTERIORI ERROR ESTIMATION – A COMPARISON OF PROCEDURES

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To address the issue of accurate and effective estimation of the discretization error of the finite element solution, the relation between different types of error estimators is investigated. The recognition of the relation between these error estimators also provides a different view point on the theory of the a posteriori error estimation and the numerical performance of the error estimators.

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